# Supporting Information

# $K_2S_2O_8$ activation by glucose at room temperature for synthesis and functionalization of heterocycles in water

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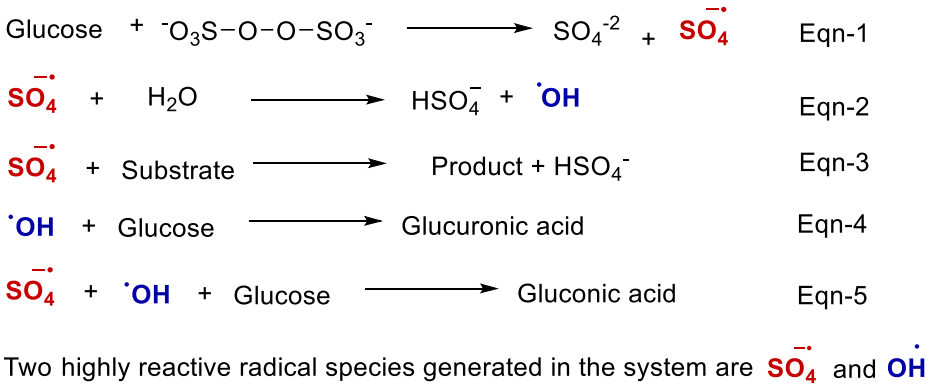
# I. MECHANISTIC INSIGHTS:

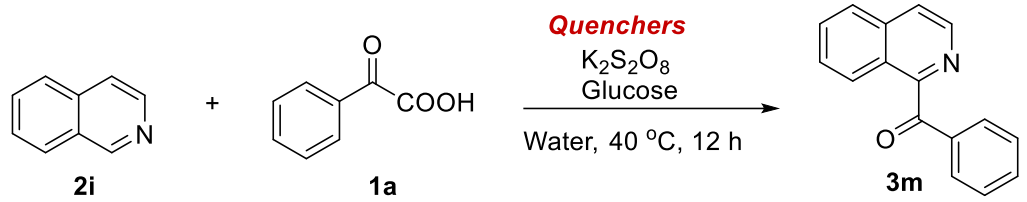
**General mechanism for $K_2S_2O_8$ activation by glucose at room temperature:**

Glucose is responsible for the heterolytic cleavage of $K_2S_2O_8$ to sulfate radical anion ($SO_4^{\bullet-}$) and sulfate anion ($SO_4^{2-}$) at room temperature (Eqn-1).[1] This $SO_4^{\bullet-}$ can further generate hydroxyl ($HO^{\bullet}$) radical by reaction with water at room temperature (Eqn-2).[1] Unlike $K_2S_2O_8$ mediated transformation in an organic solvent, two reactive radicals are present in $K_2S_2O_8$ mediated transformation in water. The $SO_4^{\bullet-}$ could alone perform the transformation depending on the nature of substrate (Eqn-3). The $HO^{\bullet}$ radical could oxidize glucose into glucuronic acid by oxidizing $-CH_2OH$ group of glucose (Eqn-4). Similarly, the presence of $SO_4^{\bullet-}$ and $HO^{\bullet}$ radical are responsible for the oxidation of –CHO group of glucose to form gluconic acid (Eqn-5).[2] However, the two radicals could work synergistically with the substrate, which is clearly distinct from the reactions performed in an organic solvent.




To understand the role of both these radicals in the oxidative transformations, we carried out some control experiments. As reported in the literature,[3] some solvents and organic compounds are used to quench the radicals. Under the optimized condition, isoquinoline was acylated in

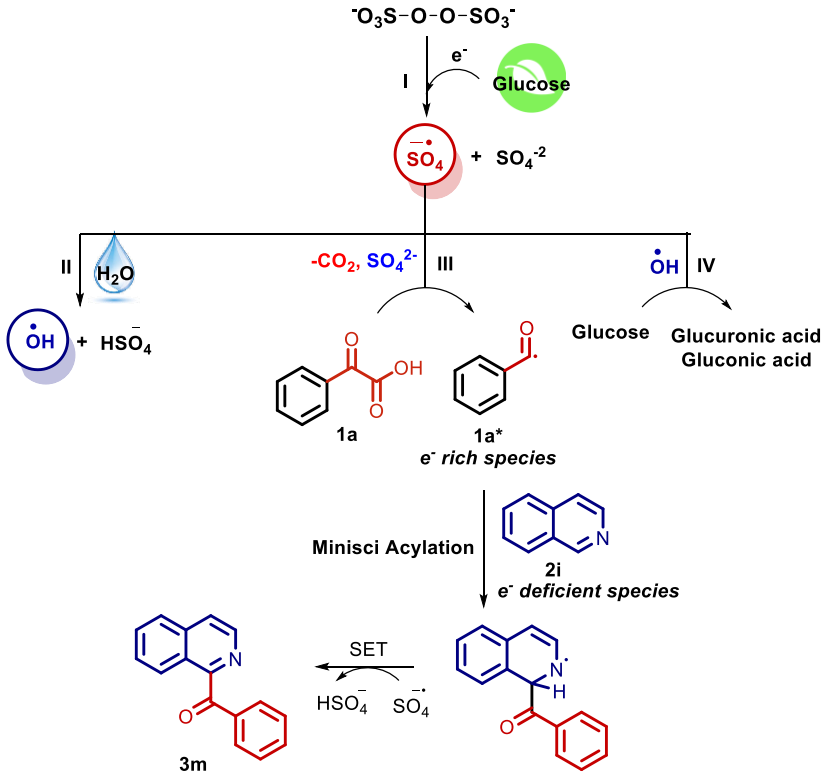
85% yield (Entry-1). When water was replaced with methanol, a solvent known to quench $SO_4^{\bullet-}$, no product formation was observed (Entry-2). However, when methanol was added as a quencher in the optimized condition, the product **3m** formed in 20% yield, suggesting the role of $HO^{\bullet}$ radical as well (Entry-3). Furthermore, when a $HO^{\bullet}$ radical quencher, *tert*-butanol was added in the optimized reaction condition, the product formation was deprived to 40% yield (Entry-4). Also, *tert*-butanol along with 1 equiv of 0.1 N NaOH in the optimized reaction condition yielded reduced product (30% yield, Entry-5). As nitrobenzene is known to trap the $HO^{\bullet}$ radical, addition of 1 equiv of nitrobenzene reduced the product formation to 20% suggesting involvement of $HO^{\bullet}$ radical also in the transformation (Entry-6).




| Entry | Quencher | Radical quenched | Observation |
|---|---|---|---|
| 1 | -- | -- | **3m** – 85% yield |
| 2 | Methanol as solvent (No water) | $SO_4^{\bullet-}$ | no product formation |
| 3 | Methanol | $SO_4^{\bullet-}$ | **3m** observed in 20% yield |
| 4 | *t*-butanol | $HO^{\bullet}$ | **3m** observed in 40% yield |
| 5 | *t*-butanol + 0.1 N NaOH | $HO^{\bullet}$ | **3m** observed in 30% yield |

| | | | |
|---|---|---|---|
| 6 | Nitrobenzene | $HO^{\bullet}$ | **3m** observed in 20% yield |

From the above experiments, it cannot be claimed that only sulfate radical anion is responsible for the respective transformation. Both $SO_4^{\bullet-}$ and $HO^{\bullet}$ radicals could work synergistically for the respective oxidative transformations for the synthesis and functionalization of N-heterocycles. Based on previous reports, a mechanism of aroylation of isoquinoline is shown below:

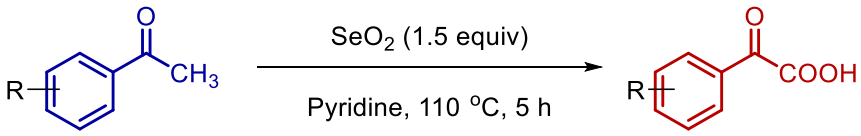


## II. EXPERIMENTAL SECTION:

### General Methods

Unless noted otherwise, all reagents and solvents were purchased from commercial sources and used as received. All reactions were performed in a screw-capped vial. Reactions were monitored by TLC, which was performed with 0.2 mm Merck pre-coated silica gel 60 F254 Aluminium sheets. TLC plates were visualized with UV light and iodine chamber. Column chromatography was performed using silica gel (60-120 mesh, 100-200 mesh, and 230-400 mesh). The $^{1}H$ and $^{13}C$ NMR spectra were obtained in $CDCl_3$, MeOD or DMSO-$d_6$ as solvent using a 400 MHz, 500 MHz and 100, 125 MHz spectrometer respectively with $Me_4Si$ as an internal standard. Chemical shifts (δ) are given in ppm and Coupling constants (*J* values) are given in Hz, pattern was designated as s, singlet; bs, broad singlet; d, doublet; dd, doublet of doublet; dt, triplet of doublet; t, triplet; m, multiplet.

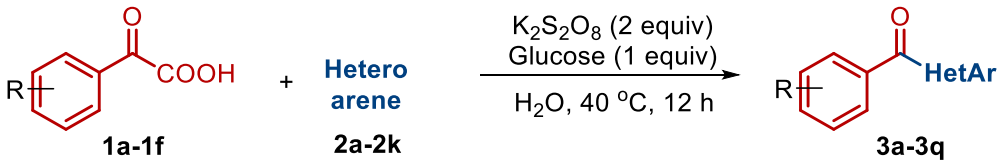
### 1. Preparation of substituted *α*-oxocarboxylic acids:




All substituted *α*-oxocarboxylic acids were prepared from oxidation of corresponding methyl ketones with $SeO_2$ according to the reported procedure.[4] In a dry, single-neck, 25-mL, round-bottom flask equipped with a stir bar and flushed with nitrogen, the substituted aryl-methyl ketone (1.0 mmol) and selenium dioxide ($SeO_2$, 1.5 equiv) were added followed by anhydrous pyridine (10 mL). The reaction mixture was heated in an oil bath to 110 °C for 1 h, and then the bath temperature was reduced to 90 °C. The mixture was stirred at this temperature (90 °C) for an additional

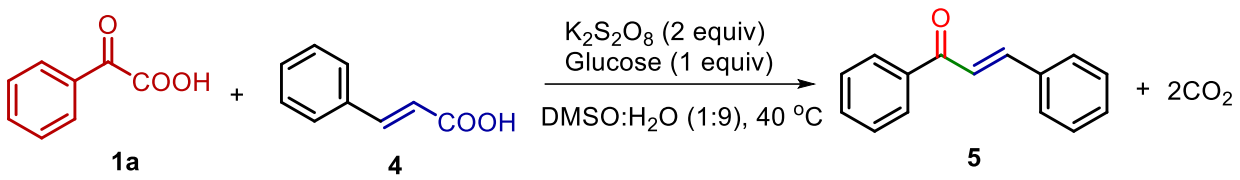
4 h, and progress of the reaction was monitored by TLC. After completion of the reaction, as determined by TLC, the solution containing precipitated selenium was filtered using a Buckner funnel, and the residue was washed with ethyl acetate (50 mL). The combined filtrate was treated with 1 N HCl (20 mL), the organic layer was separated, and the aqueous layer was extracted with ethyl acetate (3 x 50 mL). The organic layers were combined and treated with 1N NaOH (50 mL), and the aqueous layer was separated. The organic layer was extracted with water (25 mL) and the combined aqueous layers were acidified using 1N HCl to about pH 1.5. The mixture was extracted with ethyl acetate (3 x 50 mL), and the combined organic layers were dried (anhydrous $Na_2SO_4$) and concentrated on a rotary evaporator (Bath temperature: 40–45 $^oC$). The crude arylglyoxylic acid products were purified by silica-gel column chromatography using ethyl acetate:hexane (ratio: 9:1) as solvent system for elution.

**2. Procedure for the synthesis of 2-aroylated heterocycles (3a-3q):**



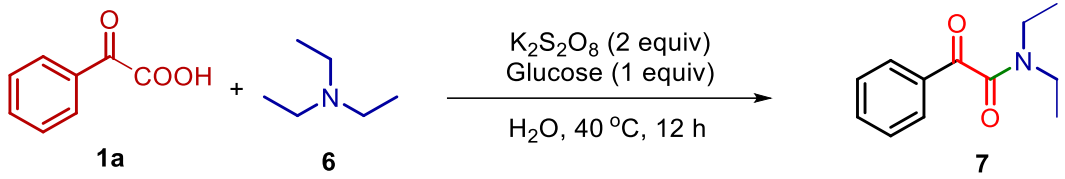

In an oven-dried screw cap vial equipped with a magnetic stir bar was charged with $\alpha$-oxocarboxylic acids derivative (0.5 mmol), heteroarenes (1 equiv), $K_2S_2O_8$ (2 equiv) and Glucose (1 equiv). Water (2 mL) was added by syringe. The tube was sealed and the mixture was allowed to stir at room temperature (almost 40 $^oC$) for 12 h. The reaction mixture was neutralized with saturated solution of $Na_2CO_3$ (10 mL) by constant stirring. It was then extracted with EtOAc (20 mL x 2). The organic layer was dried ($Na_2SO_4$), concentrated under reduced pressure, and purified by column chromatography [100-200# silica, EtOAc - hexanes = 2:8] to give the desired acylated products. *Note: 0.1 N NaOH (1 equiv) was added in some cases.*

**3. Procedure for the synthesis of E-Chalcone (5):**




To a 10 mL Schlenk tube was added Phenylglyoxylic acid (0.5 mmol), cinnamic acid (1 equiv), $K_2S_2O_8$ (2 equiv), 0.1 N NaOH (1 equiv) and Glucose (1 equiv). The tube was evacuated and backfilled with $N_2$. $H_2O$ (1.7 mL) and DMSO (0.3 mL) were added. The reaction mixture was stirred at 40 °C for 15 h. Upon completion, the resulting mixture was neutralized with saturated solution of $Na_2CO_3$ (10 mL) and the resulting mixture was extracted with EtOAc (20 mL x 2). The organic phase was separated, dried over anhydrous $Na_2SO_4$, filtered, and concentrated in *vacuo*. The resulting residue was purified by column chromatography on silica gel [100-200# silica, EtOAc - hexanes = 1:9] to give the desired product *E*-chalcone in yellow solid (87 mg, 84%).

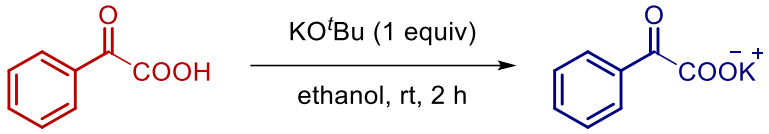
**4. Procedure for the synthesis of α-ketoamide (7):**




A sealable reaction tube equipped with a magnetic stirrer bar was charged with α-keto acid (0.5 mmol), triethylamine (3 equiv), $K_2S_2O_8$ (2 equiv) 0.1 N NaOH (1 equiv) and Glucose (1 equiv) in water (2 mL). The reaction was carried out at room temperature (~40 °C) for 12 h. Then the

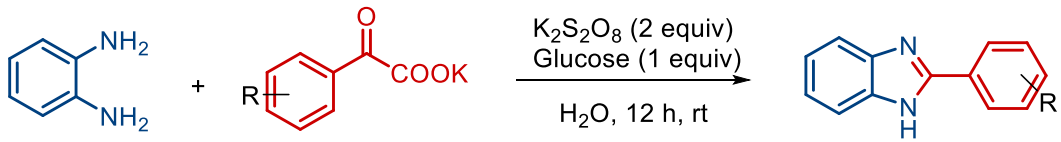
mixture was extracted with ethyl acetate (20 mL x 2). The organic phase was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel [100-200# silica, EtOAc - hexanes = 1:9] to afford the corresponding product in yellow oil (71 mg, 70%).

**5. General procedure for the synthesis of potassium salts of the α-oxocarboxylic acids (11a-11d):**



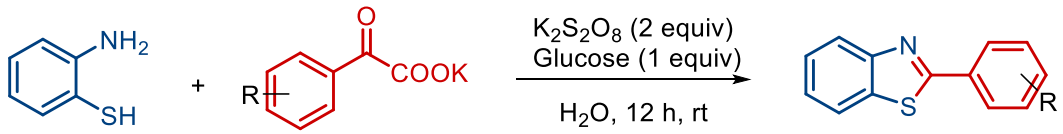

Following a literature procedure, a solution of potassium *tert*-butoxide (1 mmol) in ethanol (1 mL) was added drop by drop to a solution of α-oxocarboxylic acids (1 mmol) in ethanol (1 mL) over 30 minutes. After complete addition, the reaction mixture was stirred for another 2 h at room temperature. A gradual formation of a precipitate was observed. The resulting solid was collected by filtration, washed with ethanol (2 x 10.0 mL), diethyl ether (10.0 mL) respectively, transferred to a round-bottomed flask and dried it under vacuum to give corresponding potassium salts of *α*-oxocarboxylic acids.[5]

**6. Procedure for the synthesis of 2-arylated benzimidazoles (12a, 12d):**



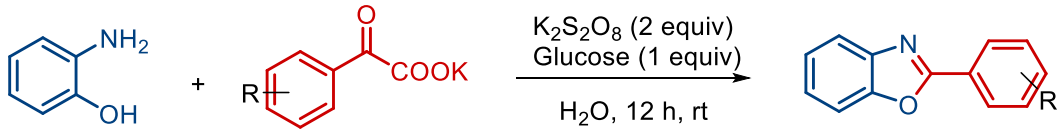
In an oven-dried screw cap sealed tube equipped with a magnetic stir bar was charged with o-phenylenediamine (0.5 mmol), aryl $\alpha$-oxocarboxylic acid salt (1 equiv), $K_2S_2O_8$ (2 equiv), Glucose (1 equiv) and water (2 mL) were added in the sealed tube. The tube was sealed and the mixture was allowed to stir at room temperature (~40 $^oC$) for 12 h. After reaction was complete, the reaction mixture was extracted with EtOAc (20 mL x 3). The organic layer was dried over sodium sulphate, concentrated under reduced pressure and purified by using column chromatography (100-200 # silica, EtOAc – Hexane = 3:7) to give the desired cyclized product.

**7. Procedure for the synthesis of 2-arylated benzothiazoles (12b, 12e):**



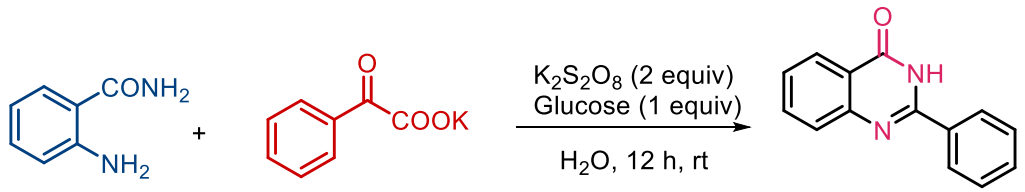

In an oven-dried screw cap sealed tube equipped with a magnetic stir bar was charged with 2-aminothiophenol (0.5 mmol), aryl $\alpha$-oxocarboxylic acid salt (1 equiv), $K_2S_2O_8$ (2 equiv), Glucose (1 equiv) and water (2 mL) were added in the sealed tube. The tube was sealed and the mixture was allowed to stir at room temperature (~40 $^oC$) for 12 h. After reaction was complete, the reaction mixture was extracted with EtOAc (20 mL x 3). The organic layer was dried over sodium sulphate, concentrated under reduced pressure and purified by using column chromatography (100-200 # silica, EtOAc – Hexane = 3:7) to give the desired cyclized product.

**8. Procedure for the synthesis of 2-arylated benzoxazoles (12c, 12f):**



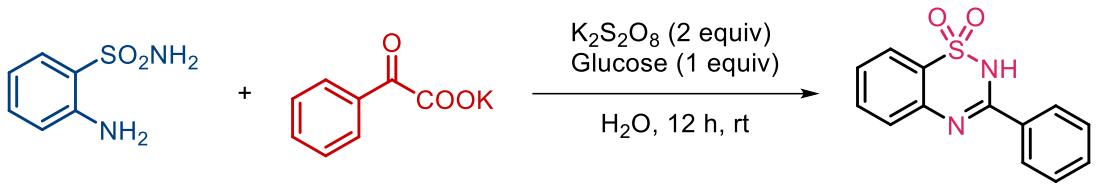
In an oven-dried screw cap sealed tube equipped with a magnetic stir bar was charged with 2-aminophenol (0.5 mmol), aryl *α*-oxocarboxylic acid salt (1 equiv), $K_2S_2O_8$ (2 equiv), Glucose (1 equiv) and water (2 mL) were added in the sealed tube. The tube was sealed and the mixture was allowed to stir at room temperature (~40 $^oC$) for 12 h. After reaction was complete, the reaction mixture was extracted with EtOAc (20 mL x 3). The organic layer was dried over sodium sulphate, concentrated under reduced pressure and purified by using column chromatography (100-200 # silica, EtOAc – Hexane = 3:7) to give the desired cyclized product.

**9. Procedure for the synthesis of 2-arylated quinazolinones (12g):**



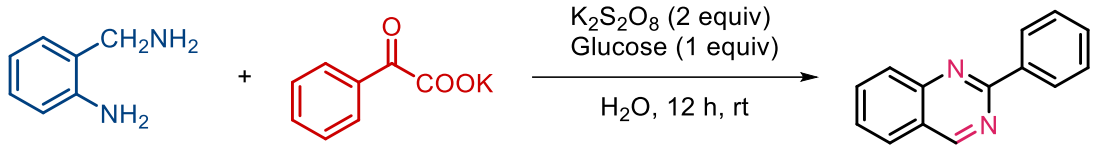

In an oven-dried screw cap sealed tube equipped with a magnetic stir bar was charged with 2- aminobenzamide derivatives (0.5 mmol), aryl *α*-oxocarboxylic acid salt (1 equiv), $K_2S_2O_8$ (2 equiv), Glucose (1 equiv) and water (2 mL) were added in the sealed tube. The tube was sealed and the mixture was allowed to stir at room temperature (~40 $^oC$) for 12 h. After reaction was complete, the reaction mixture was extracted with EtOAc (20 mL x 3). The organic layer was dried over sodium sulphate, concentrated under reduced pressure and purified by using column chromatography (100-200 # silica, EtOAc – Hexane = 3:7) to give the desired cyclized product in a yellow solid (98 mg, 89%).

**10. Procedure for the Synthesis of 2H-1,2,4-benzothiadiazine-1,1-dioxide (12h):**



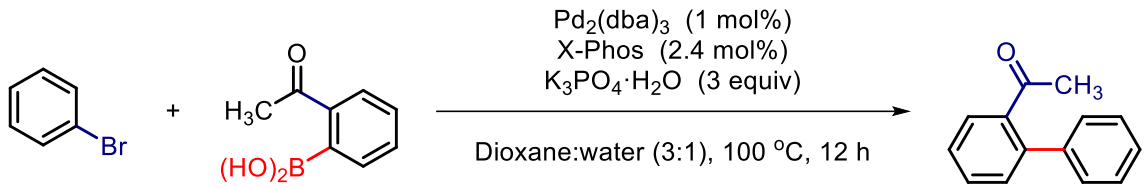

In an oven-dried sealed tube, 2-aminobenzenesulphonamide (0.5 mmol), phenylglyoxylate salt (1 equiv), $K_2S_2O_8$ (2 equiv), 0.1 N NaOH (1 equiv), Glucose (1 equiv) and water (2 mL) were added in the sealed tube. The tube was sealed and the mixture was allowed to stir at 40 $^oC$ for 12 h. After reaction was complete, the reaction mixture was extracted with EtOAc (20 mL x 3). The organic layer was dried over sodium sulphate, concentrated under reduced pressure and purified by using column chromatography (100-200 # silica, EtOAc – Hexane = 3:7) to give the desired cyclized product in a dark yellow solid (97 mg, 75%).

**11. Procedure for Synthesis of 2-Aryl Quinazoline from salt of *α*-oxocarboxylic acid and Amine (12i):**

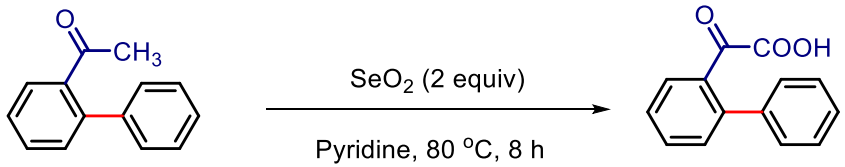



2-aminobenzylamine (0.5 mmol), salt of α-oxocarboxylic acid (1 equiv), potassium persulphate (3 equiv), 0.1 N NaOH (1 equiv) and glucose (1 equiv) were dissolved in 2 mL of water in an oven dried seal tube and stirred the reaction at room temperature for 12 h. After completion of reaction, the reaction mixture was extracted with EtOAc (20 mL x 3) and dried over sodium sulphate. Removal of the solvent under vacuum afforded the crude product, which was purified by column chromatography using hexane/ethyl acetate mixture [100-200# silica, EtOAc - hexanes = 2:8] gave the corresponding pale yellow cyclic product (82 mg, 80%).

**12. Procedure for the synthesis of biaryls oxo acid (13a)[6]:**



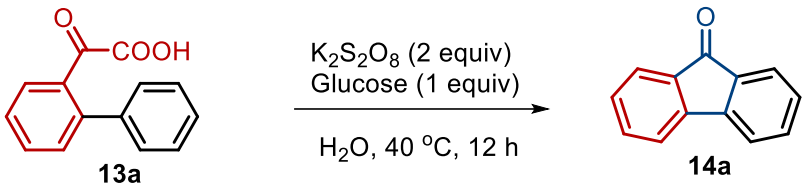

An oven-dried screw cap vial equipped with a magnetic stir bar was charged with a bromobenzene derivative (1 mmol), 2-acetyl benzeneboronic acid (1.2 equiv), $Pd_2(dba)_3$ (1 mol%), X-Phos (2.4 mol%) and $K_3PO_4 \cdot H_2O$ (3 equiv). The tube was evacuated and backfilled with nitrogen. Dioxane (3 mL) and $H_2O$ (1 mL) were added via a syringe under a flow of nitrogen. The tube was sealed and the mixture was stirred at 100 °C for 12 h. The reaction mixture was allowed to cool to room temperature, neutralized with a saturated solution of $Na_2CO_3$ (10 mL) and extracted with EtOAc (20 mL × 2). The combined organic layers were dried ($Na_2SO_4$), concentrated under reduced pressure, and purified by column chromatography [60–120# and 100–200# silica, ethyl acetate/hexane = 1 : 9] to give the desired product.




Following a literature procedure,[4] a solution of methyl ketone substrate (0.5 mmol), $SeO_2$ (2 equiv.) and pyridine (0.5 mL) was heated at 80 °C for 6–8 h. After complete consumption of the substrate (monitored by TLC), the reaction mixture was filtered through a Buchner funnel and the residue was washed with ethyl acetate. The organic layer was extracted with 1 N HCl (10 mL × 2). The organic layer was separated and extracted with a 2 M NaOH solution (10 mL × 2). The combined aqueous layer was separated and acidified with 6 N HCl to adjust the pH to 2. The aqueous

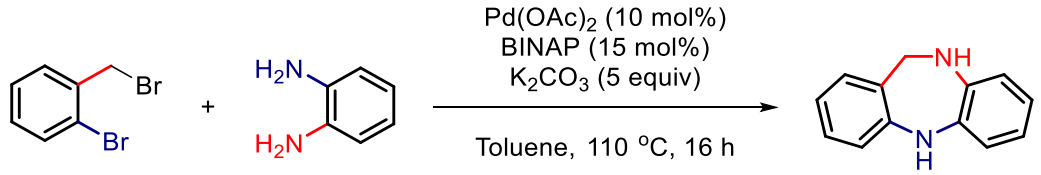
layer was extracted with ethyl acetate (20 mL × 2). The combined organic layers were concentrated under reduced pressure and purified by recrystallization (dichloromethane/hexane) to give the desired product.

**13. Procedure for the synthesis of 9-fluorenone (14a):**



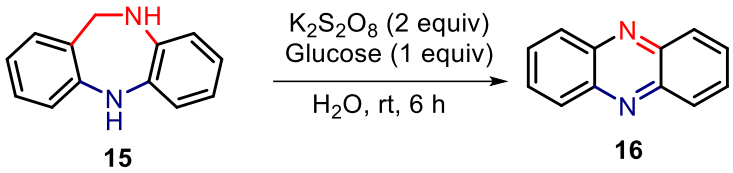

In an oven-dried screw cap vial equipped with a magnetic stir bar was charged with biaryls α-keto acid (0.5 mmol), $K_2S_2O_8$ (2 equiv), Glucose (1 equiv) and $H_2O$ (2 mL). The tube was sealed and the mixture was allowed to stir at room temperature (~40 °C) for 12 h. The reaction mixture was neutralized with saturated solution of $Na_2CO_3$ (10 mL) and extracted with EtOAc (20 mL x 2). The organic layers were dried ($Na_2SO_4$), concentrated under reduced pressure, and purified by column chromatography [100-200# silica, ethyl acetate/hexane = 1:9] to give the desired cyclized product in yellow solid (64 mg, 71%).

**14. General Procedure for the Synthesis of Dibenzodiazepines (15)[7]:**



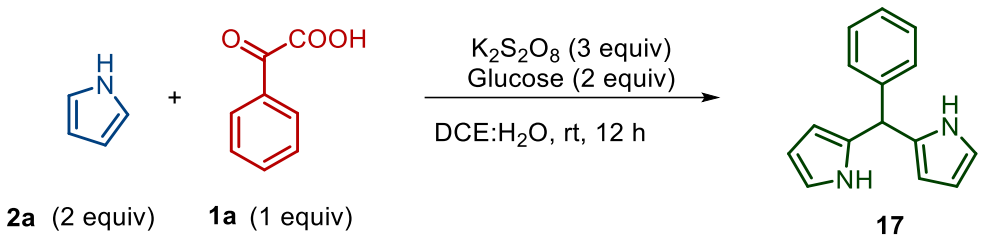
Following a literature procedure, a mixture of *o*-phenylenediamine (1.5 mmol), 2-bromobenzyl bromide (1 mmol), $Pd(OAc)_2$ (10 mol%), BINAP (15 mol%), and $K_2CO_3$ (5 equiv) in toluene (6 mL) was purged with argon and heated at 110 °C for 16 h in a rubber septum-covered screw-capped vial under argon. The reaction mixture was cooled to room temperature and diluted with excess ethyl acetate. The resulting suspension was filtered through a Celite pad, and the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 4:1–3:2) to give the dibenzodiazepines.

**15. Procedure for the synthesis of Phenazine from Dibenzodiazepine (16):**



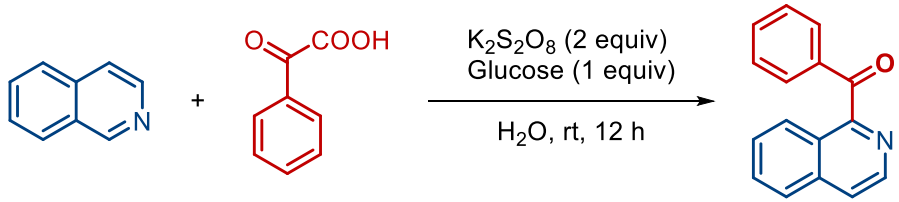

A stirred suspension of dibenzodiazepine (0.5 mmol), $K_2S_2O_8$ (2 equiv) and Glucose (1 equiv) in water (2 mL) was stirred at room temperature (~40 $^oC$) for 6 h in a screw-cap vial. Then the mixture was extracted with ethyl acetate (20 mL x 2). The organic phase was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using hexane/ethyl acetate as eluent [100-200# silica, EtOAc - hexanes = 1:9] to give phenazine in light yellow solid (78 mg, 87%).

**16. Procedure for the synthesis of 5-phenyl dipyrromethane (17):**




In an oven-dried screw cap vial equipped with a magnetic stir bar, phenylglyoxylic acid (0.5 mmol) was dissolved in water (2 mL). Pyrrole (2 equiv), $K_2S_2O_8$ (3 equiv) and Glucose (2 equiv) were then added in the tube. The tube was sealed and the mixture was allowed to stir at room temperature (~40 $^oC$) for 12 h. The reaction mixture was neutralized with saturated solution of $NaHCO_3$ (10 mL) by constant stirring. It was then extracted with DCM (20 mL x 3). The organic layer was dried ($Na_2SO_4$), concentrated under reduced pressure, and purified by column chromatography [100-200# silica, EtOAc - hexanes = 1:9] to give the desired product in dark brown solid (56 mg, 51%).

**17. Procedure for scale up synthesis of 1-benzoyl isoquinoline (3m):**

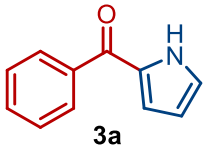



In an oven-dried 250 mL round bottom flask equipped with a magnetic stir bar, isoquinoline (0.78 g, 6 mmol), Phenyglyoxylic acid (0.90 g, 1 equiv), $K_2S_2O_8$ (3.24 g, 2 equiv) and Glucose (1.08 g, 1 equiv) were added. Water (25 mL) was added and the reaction was stirred at 40 $^oC$ for 12 h. After completion of reaction, the reaction mixture was neutralized with saturated solution of $Na_2CO_3$ (20 mL) by constant stirring. It was then

extracted with EtOAc (30 mL x 2). The organic layer was dried ($Na_2SO_4$), concentrated under reduced pressure, and purified by column chromatography [100-200# silica, EtOAc - hexanes = 2:8] to give **1**-benzoyl isoquinoline (1.10 g, 80%).

## III. CHARACTERIZATION DATA:

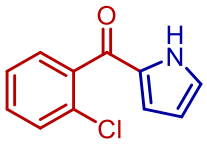
***Phenyl(1H-pyrrol-2-yl)methanone (3a)***[8] Brown solid (68 mg, 80%)




**3a**

$^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ 10.16 (s, 1H), 7.90 (d, *J* = 7.1 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.17 (s, 1H), 6.89 (s, 1H), 6.35-6.34 (m, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 185.1, 138.4, 133.5, 131.9, 131.2, 130.2, 129.1, 128.5, 128.4, 125.6, 119.9, 111.1

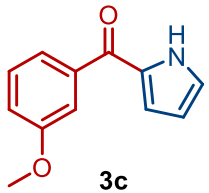
***(2-chlorophenyl)(1H-pyrrol-2-yl)methanone (3b)***[8] Yellow solid (76 mg, 75%)




**3b**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 10.56 (s, 1H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.43 (td, *J* = 1.7, 7.0 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.24 (s, 1H), 6.64 (s, 1H), 6.33-6.31 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 184.8, 138.1, 133.2, 131.6, 131.3, 130.9, 130.5, 130.3, 129.4, 129.3, 127.3, 126.7, 126.6, 126.3, 121.5, 111.4

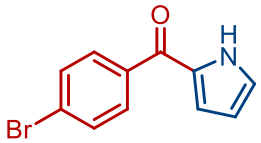
***(3-methoxyphenyl)(1H-pyrrol-2-yl)methanone (3c)***[8] Dark Yellow solid (73 mg, 73%)




**3c**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.91 (s, 1H), 7.52 (d, $J$ = 7.5 Hz, 1H), 7.44-7.39 (m, 2H), 7.18 (s, 1H), 7.13 (dd, $J$ = 2.4, 8.2 Hz, 1H), 6.94 (s, 1H), 6.37 (s, 1H), 3.90 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 184.6, 159.6, 139.6, 131.1, 129.3, 125.4, 121.5, 119.5, 118.2, 113.6, 111.1, 55.5

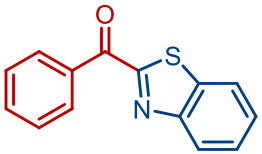
***(4-bromophenyl)(1H-pyrrol-2-yl)methanone (3d)***[8] Dark brown solid (95 mg, 77%)




**3d**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.89 (s, 1H), 7.80 (dd, $J$ = 1.8, 6.6 Hz, 2H), 7.65 (dd, $J$ = 1.8, 6.7 Hz, 2H), 7.20-7.18 (m, 1H), 6.89-6.87 (m, 1H), 6.38-6.36 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 183.5, 137.0, 131.6, 130.8, 130.5, 126.7, 125.5, 119.3, 111.3

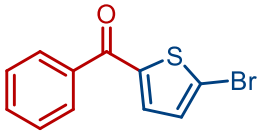
***Benzo[d]thiazol-2-yl(phenyl)methanone (3e)***[8] Light brown solid (83 mg, 70%)




**3e**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.60-8.57 (m, 2H), 8.28-8.26 (m, 1H). 8.06-8.04 (m, 1H), 7.72-7.68 (m, 1H), 7.64-7.59 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 185.4, 167.1, 153.9, 137.0, 134.9, 133.9, 131.3, 128.5, 127.6, 126.9, 125.7, 122.2.

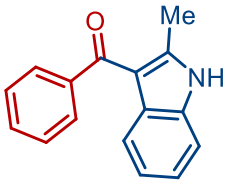
***(5-bromothiophen-2-yl)(phenyl)methanone (3f)***[8] Light brown solid (103 mg, 78%)




**3f**

$^{1}$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.08 (d, $J$ = 5.1 Hz, 1H), 7.78 (d, $J$ = 8.3 Hz, 2H), 7.75 (t, $J$ = 7.4 Hz, 1H), 7.57 (t, $J$ =7.5 Hz, 2H), 7.36 (d, $J$ = 5.2 Hz, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 187.9, 137.9, 135.4, 134.1, 133.7, 133.2, 129.7, 129.5, 129.3, 129.1, 115.7

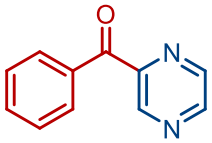
***(2-methyl-1H-indol-3-yl)(phenyl)methanone (3g)***[8] Yellow solid (80 mg, 68%)




**3g**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.77 (s, 1H), 7.78 (d, $J$ = 7 Hz, 2H), 7.57 (t, 7.4 Hz, 1H), 7.48 (t, $J$ = 7.3 Hz, 2H), 7.41 (d, $J$ = 8.1 Hz, 1H), 7.33 (d, $J$ = 8 Hz, 1H), 7.19 (t, $J$ = 7.1 Hz, 1H), 7.09 (t, $J$ = 7.2 Hz, 1H), 2.56 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 193.3, 143.6, 141.3, 134.7, 131.5, 128.9, 128.3, 127.6, 122.4, 121.6, 120.9, 114.0, 110.6, 96.1, 14.5

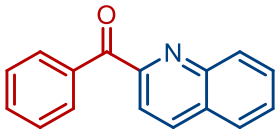
***Phenyl(pyrazin-2-yl)methanone (3j)***[9] White solid (38 mg, 40%)




**3j**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.28 (d, *J* = 1.2 Hz, 1H), 8.81 (d, *J* = 2.5 Hz, 1H), 8.72-8.71 (m, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 192.3, 146.8, 146.1, 142.9, 133.6, 130.9, 128.4

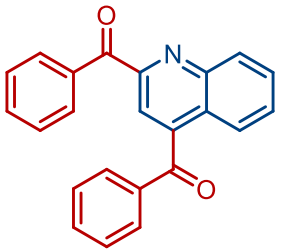
***Phenyl(quinolin-2-yl)methanone (3k)***[10] White solid (70 mg, 60%)




**3k**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.37 (d, *J* = 8.5 Hz, 1H), 8.27-8.22 (m, 3H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.93 (dd, *J* = 0.7, 8.1 Hz, 1H), 7.83-7.78 (m, 1H), 7.70-7.63 (m, 2H), 7.54 (t, *J* = 6.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 193.8, 154.7, 146.7, 137.1, 136.2, 133.1, 131.5, 130.6, 130.1, 128.9, 128.4, 128.2, 127.7, 120.8.

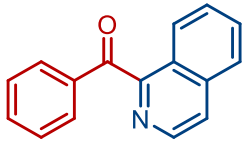
***Quinoline-2,4-diylbis(phenylmethanone) (3l)***[10] Off-white solid (50 mg, 30%)



**3l**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.34-8.28 (m, 3H), 8.15 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.93 (dd, *J* = 1.0, 8.2 Hz, 2H), 7.88-7.84 (m, 1H), 7.70-7.66 (m, 3H), 7.58-7.51 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 195.7, 193.0, 153.8, 147.2, 145.5, 136.4, 135.8, 134.4, 133.3, 131.5, 130.6, 129.6, 128.9, 128.2, 125.7, 125.4, 119.4.

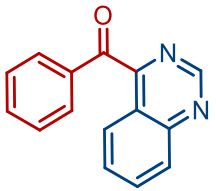
***Isoquinolin-1-yl(phenyl)methanone (3m)***[11] White solid (99 mg, 85%)



**3m**

$^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ 8.57 (d, *J* = 5.6 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 5.6 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 2H), 7.45 (t , *J* = 7.7 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 194.8, 156.4, 141.2, 136.8, 136.7, 133.7, 130.8, 128.6, 128.4, 127.2, 126.4, 126.2, 122.7

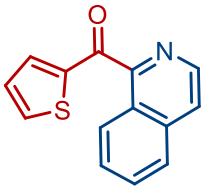
***Phenyl(quinazolin-4-yl)methanone (3n)***[12] Light brown solid (92 mg, 79%)



**3n**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.44 (s, 1H), 8.17 (d, $J$ = 8.5 Hz, 1H), 8.08 (d, $J$ = 8.4 Hz, 1H), 8.01-7.96 (m, 3H), 7.69-7.65 (m, 2H), 7.52 (t, $J$ = 7.6 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 192.8, 164.1, 153.8, 151.3, 135.2, 134.7, 134.5, 130.6, 129.1, 128.8, 128.7, 125.8, 122.1

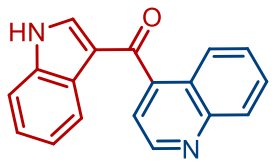
***Isoquinolin-1-yl(thiophen-2-yl)methanone (3o)***[11] Light brown solid (87 mg, 73%)



**3o**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.64 (d, $J$ = 5.6 Hz, 1H), 8.56 (d, $J$ = 8.6 Hz, 1H), 7.92-7.85 (m, 2H), 7.83 (d, $J$ = 5.6 Hz, 1H), 7.79-7.77 (m, 2H), 7.67 (td, $J$ = 1.2, 7.1 Hz, 1H), 7.17 (t, $J$ = 4.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 186.1, 154.6, 142.6, 140.9, 136.9, 136.7, 136.1, 130.7, 128.7, 128.4, 128.1, 127.1, 126.4, 126.3, 123.6

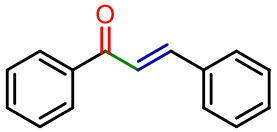
***(1H-indol-3-yl)(quinolin-4-yl)methanone (3p)***[10] Yellow solid (108 mg, 80%)




**3p**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.10 (d, *J* = 3.1 Hz, 1H), 8.83 (s, 1H), 8.68 (d, *J* = 7.7 Hz, 1H), 8.37 (d, *J* = 8.5 Hz, 1H), 8.31 (d, *J* = 8.5 Hz, 1H), 8.25 (d, *J* = 8.4 Hz, 1H), 7.93, (d, *J* = 8 Hz, 1H), 7.82 (t, *J* = 7.1 Hz, 1H), 7.67 (t, *J* = 7 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.42-7.37 (m, 2H)

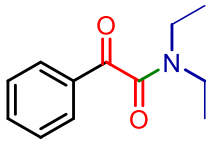
***(E)-chalcone (5)***[12] Yellow solid (87 mg, 84%)




**5**

$^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ 8.02 (d, *J* = 7.7 Hz, 2H), 7.83-7.79 (m, 1H), 7.65-7.63 (m, 2H), 7.58-7.49 (m, 4H), 7.42-7.40 (m, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 190.6, 144.9, 138.3, 134.9, 132.8, 130.6, 129.1, 128.7, 128.6, 128.5, 122.2.

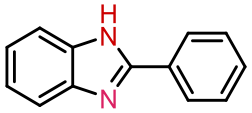
***N,N-diethyl-2-oxo-2-phenylacetamide (7)***[13] Yellow oil yield (71 mg, 70%)




**7**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.94 (d, $J$ = 8.4 Hz, 2H), 7.65–7.61 (m, 1H), 7.51 (t, $J$ = 7.7 Hz, 2H), 3.56 (q, $J$ = 7.2 Hz, 2H), 3.24 (q, $J$ = 7.1 Hz, 2H), 1.29 (t, $J$ = 7.2 Hz, 3H), 1.16 (t, $J$ = 7.1 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 191.6, 166.7, 134.5, 133.2, 129.6, 128.9, 42.1, 38.8, 14.1, 12.8.

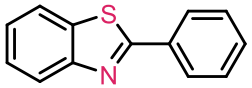
***2-phenyl-1H-benzo[d]imidazole (12a)***[14] White solid (82 mg, 85%)




**12a**

$^{1}$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 12.60 (s, 1H), 8.30 (dd, $J$ = 1.7, 7.2 Hz, 2H), 7.84 (d, $J$ = 7.9 Hz, 1H), 7.56-7.47 (m, 4H), 7.33 (t, $J$ = 8 Hz, 2H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 155.1, 154.6, 136.1, 132.5, 132.4, 130.8, 130.7, 129.7, 129.3, 128.3, 115.6.

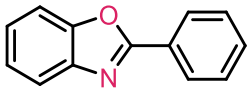
***2-phenylbenzo[d]thiazole (12b)***[14] White solid (84 mg, 80%)




**12b**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.15-8.10 (m, 3H), 7.93 (dd, $J$ = 0.4, 8 Hz, 1H), 7.56-7.50 (m, 4H), 7.41 (t, $J$ = 7.1 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 168.1, 154.1, 135.1, 133.6, 130.9, 129.0, 127.6, 126.3, 125.2, 123.3, 121.6.

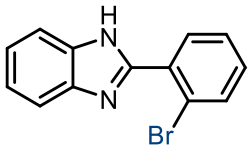
***2-phenylbenzo[d]oxazole (12c)***[14] White solid (73 mg, 75%)



**12c**

$^{1}$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.20 (dd, $J$ = 1.4, 7.1 Hz, 2H), 7.82-7.77 (m, 2H), 7.62-7.58 (m, 3H), 7.45-7.39 (m, 2H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 162.7, 150.7, 141.9, 132.4, 129.7, 127.7, 126.8, 125.9, 125.3, 123.6, 120.3, 111.4.

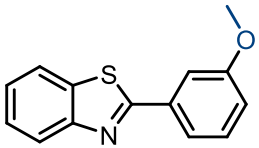
***2-(2-bromophenyl)-1H-benzo[d]imidazole (12d)***[14] White solid (103 mg, 76 %)



**12d**

$^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.67 (s, 1H), 7.82 (d, $J$ = 7.8Hz, 1H), 7.73 (d, $J$ = 7.9Hz, 1H), 7.61 (t, $J$ = 7.32, 1H), 7.55-7.49 (m, 2H), 7.45-7.33 (m, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 158.9, 154.1, 138.1, 132.9, 132.6, 132.1, 131.4, 131.3, 131.2, 129.4, 127.9, 123.9, 122.2, 115.9.

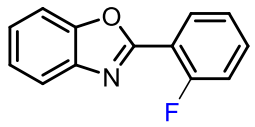
***2-(3-methoxyphenyl)benzo[d]thiazole (12e)***[14] White solid (95 mg, 79%)



**12e**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.10 (d, $J$ = 8 Hz, 1H), 7.92 (d, $J$ = 8 Hz, 1H), 7.71-7.70 (m, 1H), 7.60 (d, $J$ = 8.1 Hz, 1H), 7.54-7.50 (m, 1H), 7.43-7.39 (m, 2H), 7.06 (dd, $J$ = 8.2, 2.5 Hz, 1H), 3.94 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 167.9, 160.1, 154.1, 135.1, 134.9, 130.1, 126.3, 125.3, 121.6, 120.3, 117.4, 112.1, 55.5.

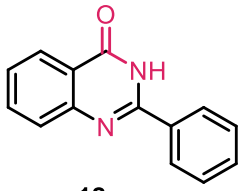
***2-(2-fluorophenyl)benzo[d]oxazole (12f)*** [14] White solid (79 mg, 75%)




**12f**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.88 (dd, $J$ = 7.9, 1.5 Hz, 1H), 7.72 (td, $J$ = 7.3, 1.7 Hz, 1H), 7.61-7.52 (m, 2H), 7.46-7.38 (m, 2H), 7.31 (td, $J$ = 7.6, 0.9 Hz, 1H), 7.23 (t, $J$ = 10 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 162.0, 159.5, 151.8, 150.7, 146.7, 132.7, 132.6, 131.9, 131.5, 131.1, 131.0, 129.7, 125.8, 124.3, 122.9, 122.8, 116.5, 116.4, 116.2.

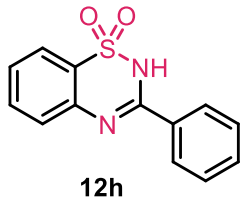
***2-phenylquinazolin-4(3H)-one (12g)*** [14] Yellow solid (98 mg, 89%)




**12g**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 11.69 (s, 1H), 8.35 (d, *J* = 7.8 Hz, 1H), 8.29-8.27 (m, 2H), 7.87-7.81 (m, 2H), 7.62-7.60 (m, 3H), 7.53 (t, *J* = 6.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 163.9, 151.7, 149.5, 134.9, 132.8, 131.7, 129.1, 128.0, 127.4, 126.8, 126.4, 120.8.

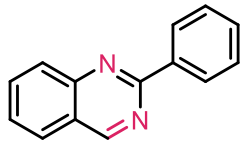
***3-phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (12h)[15]*** Dark yellow solid (97 mg, 75%)




**12h**

$^{1}$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 12.22 (s, 1H), 8.05 (d, *J* = 7.3 Hz, 2H), 7.87 (d, *J*= 7.9 Hz, 1H), 7.75-7.69 (m, 2H), 7.65-7.62 (m, 3H), 7.51 (t, *J* = 7.3 Hz, 1H).

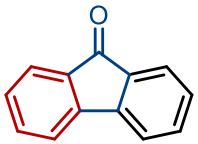
***2-phenylquinazoline (12i)[15]*** Pale yellow solid (82 mg, 80%)




**12i**

$^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ 9.47 (s, 1H), 8.61 (d, *J* = 8.5 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.93-7.89 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.55-7.50 (m, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 160.6, 150.8, 138.1, 134.2, 130.7, 128.7, 128.6, 127.4, 127.2, 123.7.

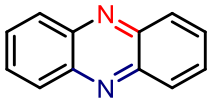
***9H-fluoren-9-one (14a)[6]*** Yellow solid (64 mg, 71%)




**14a**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.64 (dd, $J$ = 0.6, 7.2 Hz, 2H), 7.49-7.44 (m, 4H), 7.29-7.26 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 193.9, 144.4, 134.9, 134.4, 134.1, 129.3, 129.1, 124.5, 124.3, 120.3.

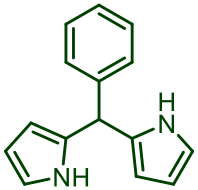
***Phenazine (16)***[16] Light yellow solid (78 mg, 87%)




**16**

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.30-8.27 (m, 4H), 7.89-7.86 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 143.5, 130.5, 129.7.

***2,2'-(phenylmethylene)bis(1H-pyrrole) (17)***[17] Dark brown solid (56 mg, 51%)




**17**

$^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.90 (s, 2H), 7.34-7.21 (m, 5H), 6.68 (s, 2H), 6.18-6.16 (m, 2H), 5.92 (s, 2H), 5.46 (s, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 142.2, 132.6, 128.7, 128.5, 127.1, 117.4, 108.5, 107.4, 44.1.

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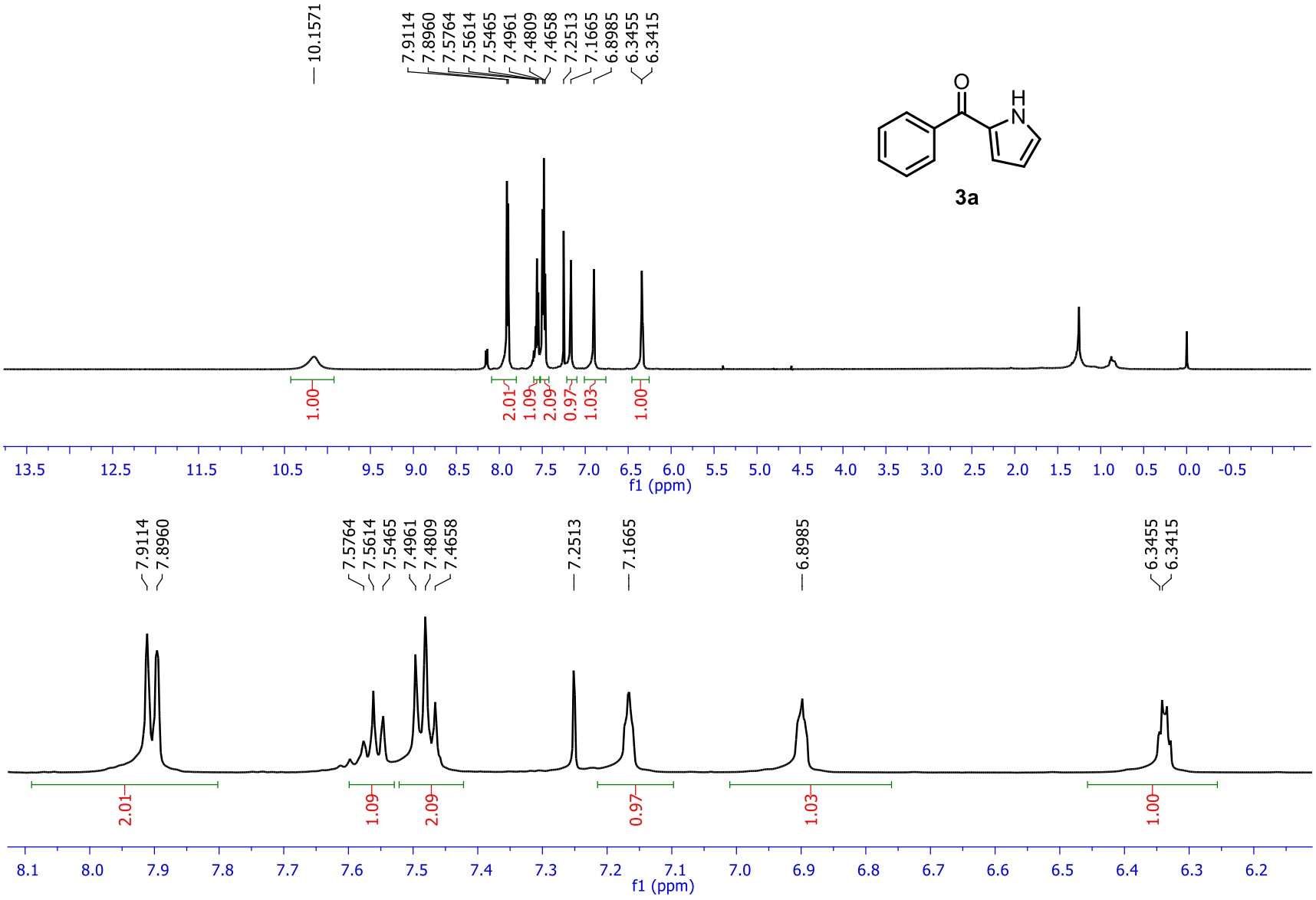
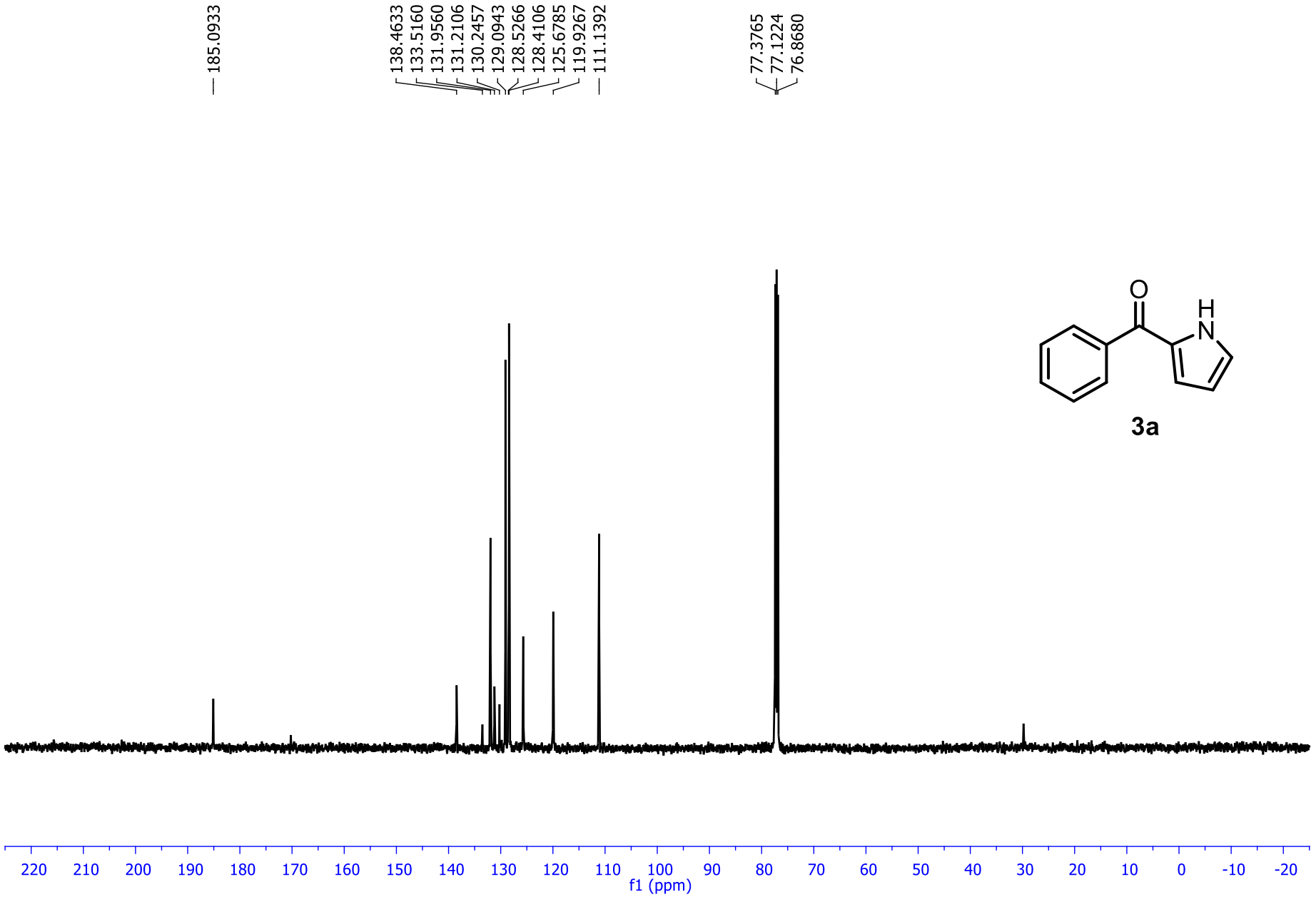
## V. $^{1}H$ AND $^{13}C$ SPECTRA

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131.2106
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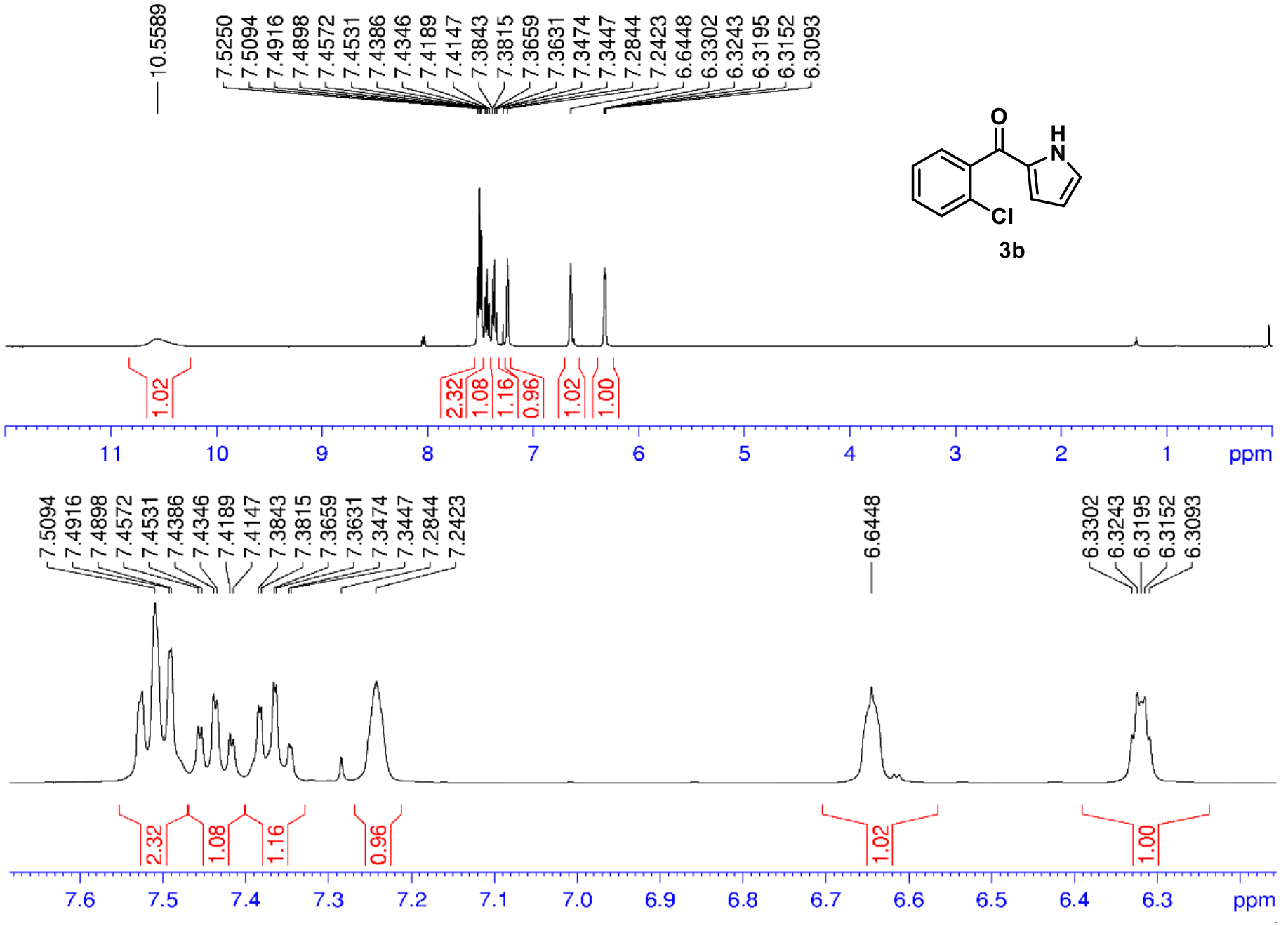
129.0943
128.5266
128.4106
125.6785
119.9267
111.1392
77.3765
77.1224
76.8680
O
H
N
3a
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.4898
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7.4531
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7.4346
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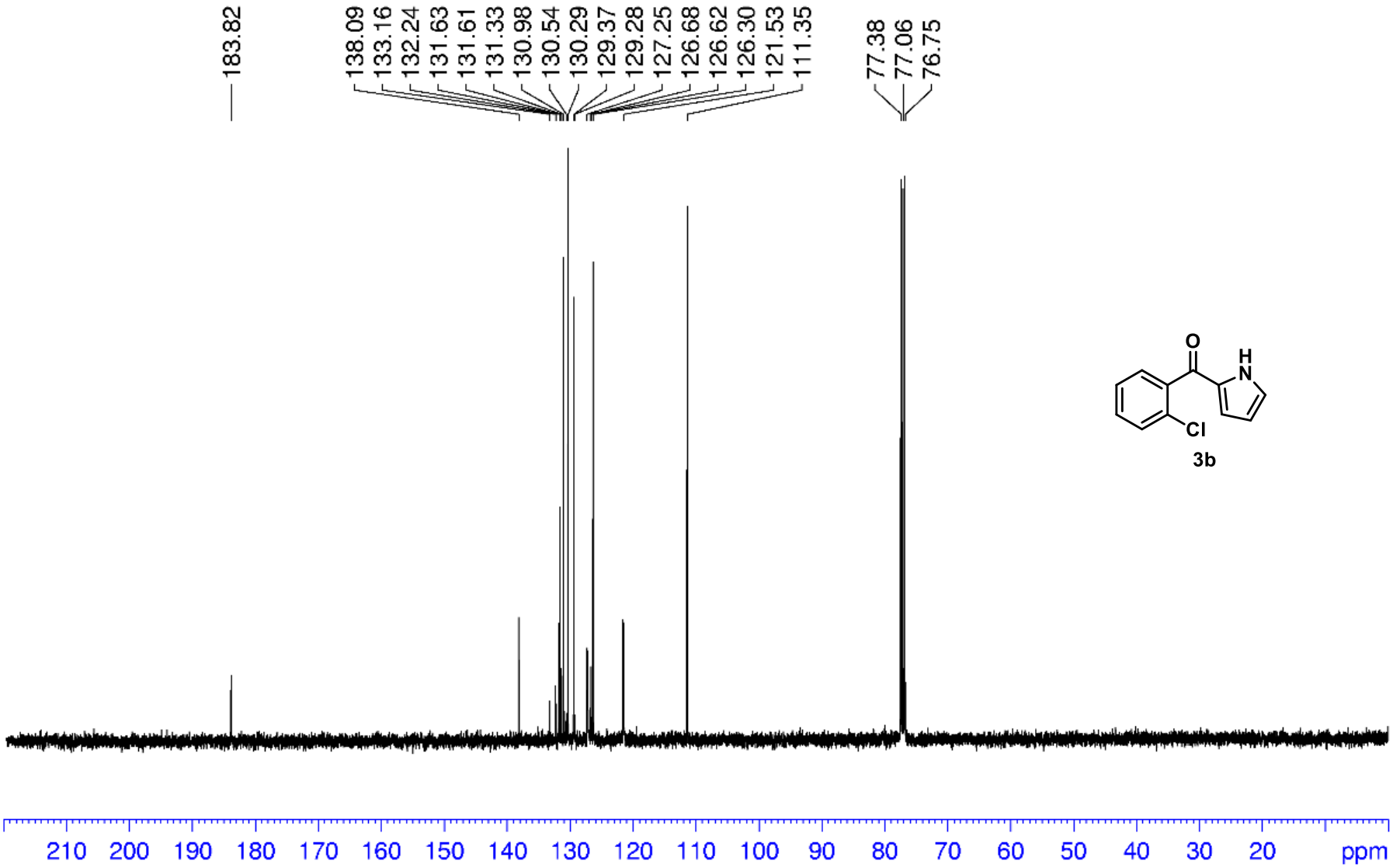
7.4147
7.3843
7.3815
7.3659
7.3631
7.3474
7.3447
7.2844
7.2423
6.6448
6.3302
6.3243
6.3195
6.3152
6.3093
O
H
N
Cl
3b
1.02
2.32
1.08
1.16
0.96
1.02
1.00
11
10
9
8
7
6
5
4
3
2
1
ppm
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
ppm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133.16
132.24
131.63
131.61
131.33
130.98
130.54
130.29
129.37
129.28
127.25
126.68
126.62
126.30
121.53
111.35
77.38
77.06
76.75
O
H
N
Cl
3b
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160
150
140
130
120
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100
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80
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60
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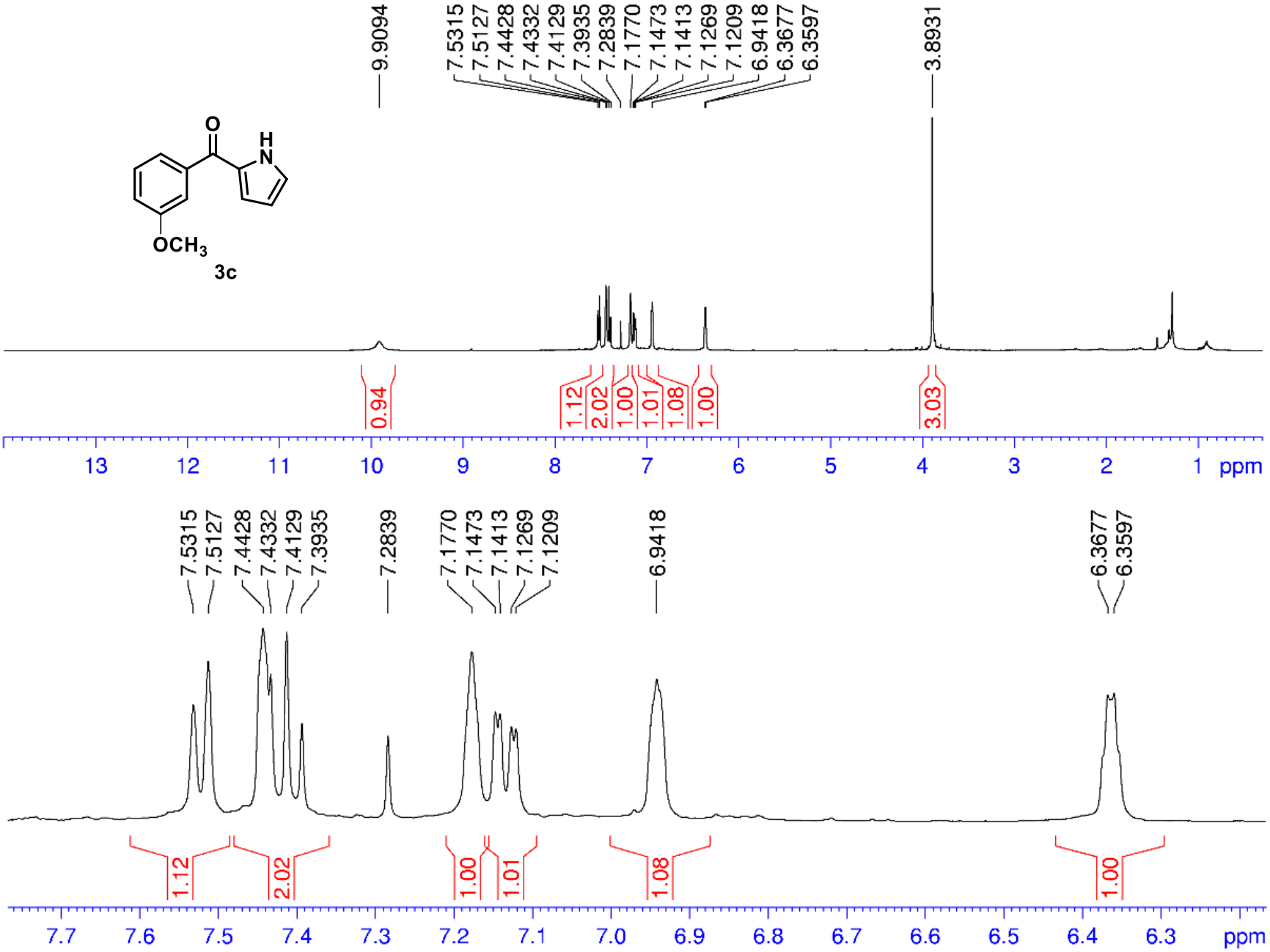
30
20
ppm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7.1413
7.1269
7.1209
6.9418
6.3677
6.3597
3.8931
O
H
N
OCH3
3c
0.94
1.12
2.02
1.00
1.01
1.08
1.00
3.03
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
7.5315
7.5127
7.4428
7.4332
7.4129
7.3935
7.2839
7.1770
7.1473
7.1413
7.1269
7.1209
6.9418
6.3677
6.3597
1.12
2.02
1.00
1.01
1.08
1.00
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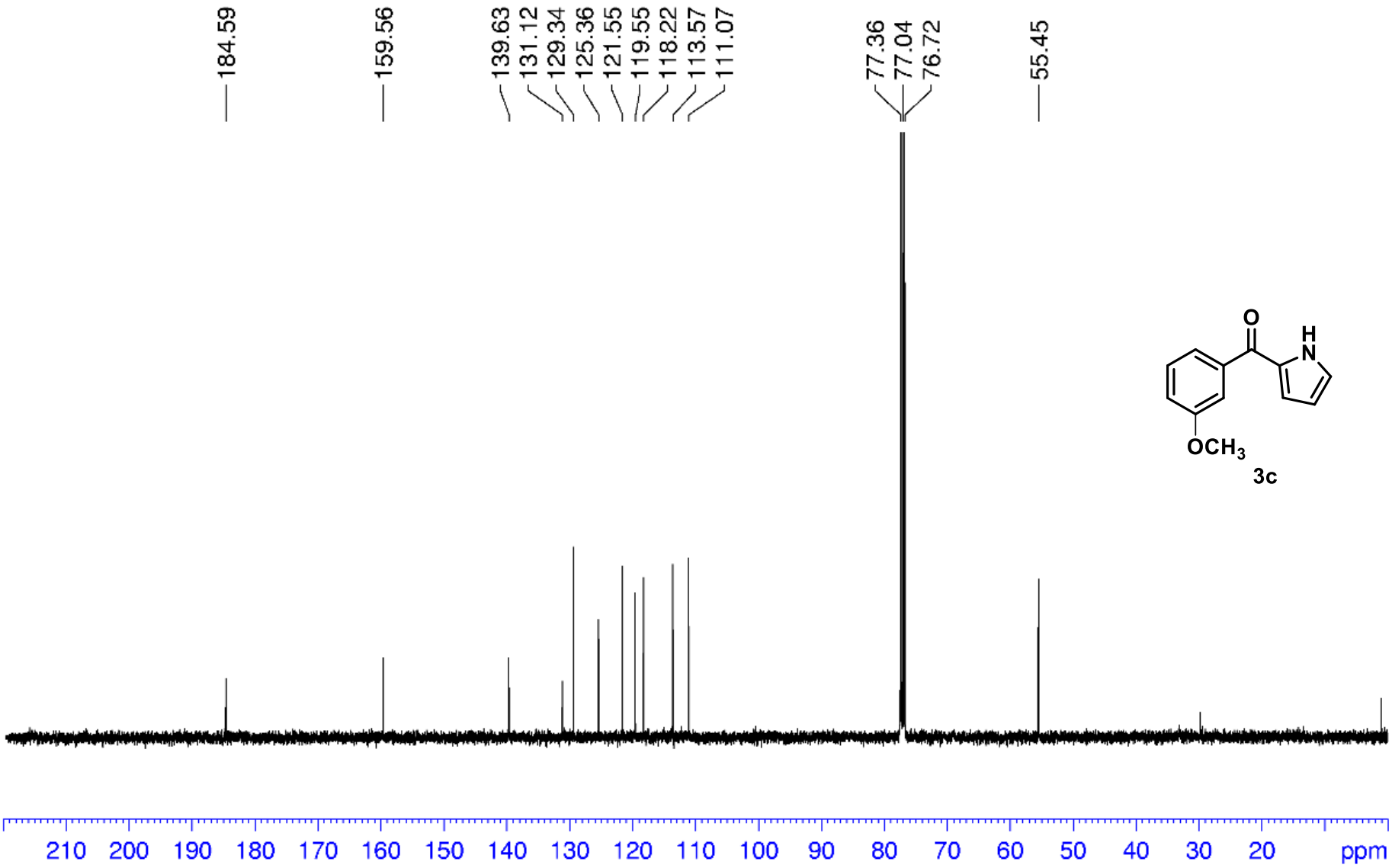
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119.55
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77.04
76.72
55.45
O
H
N
OCH3
3c
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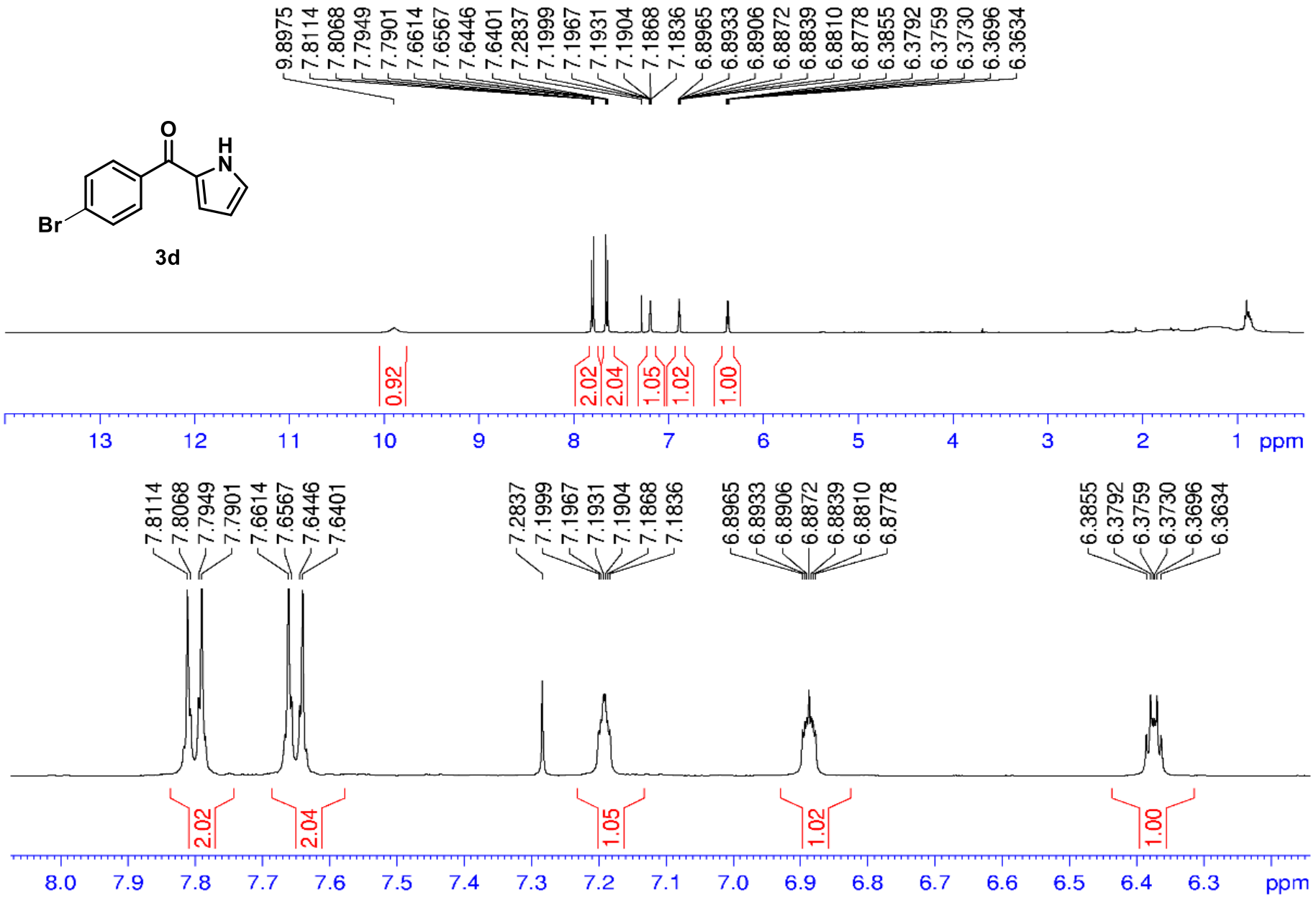
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7.1967
7.1931
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6.8839
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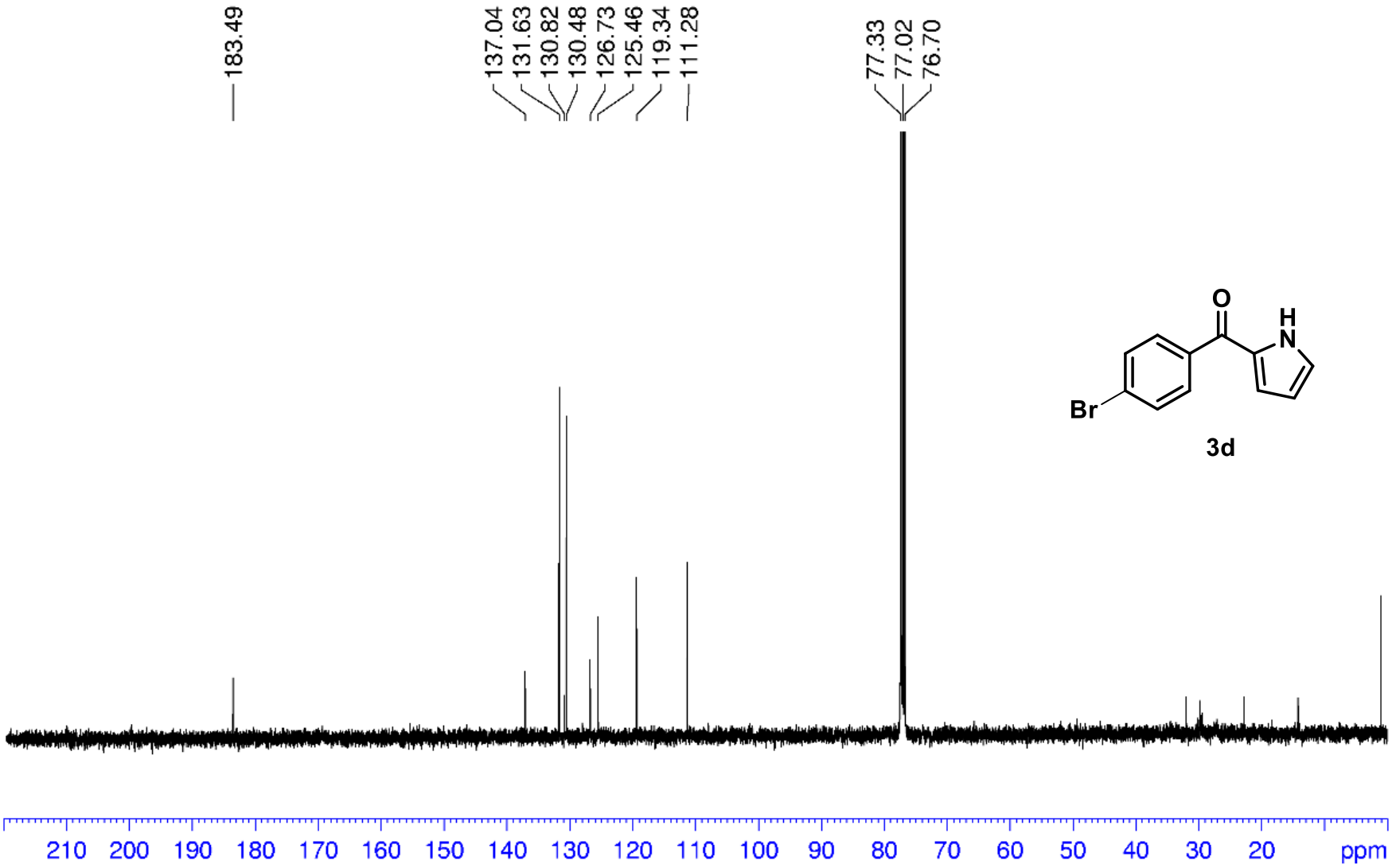
6.8778
6.3855
6.3792
6.3759
6.3730
6.3696
6.3634
O
H
N
Br
3d
0.92
2.02
2.04
1.05
1.02
1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
2.02
2.04
1.05
1.02
1.00
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 ppm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H
N
Br
3d
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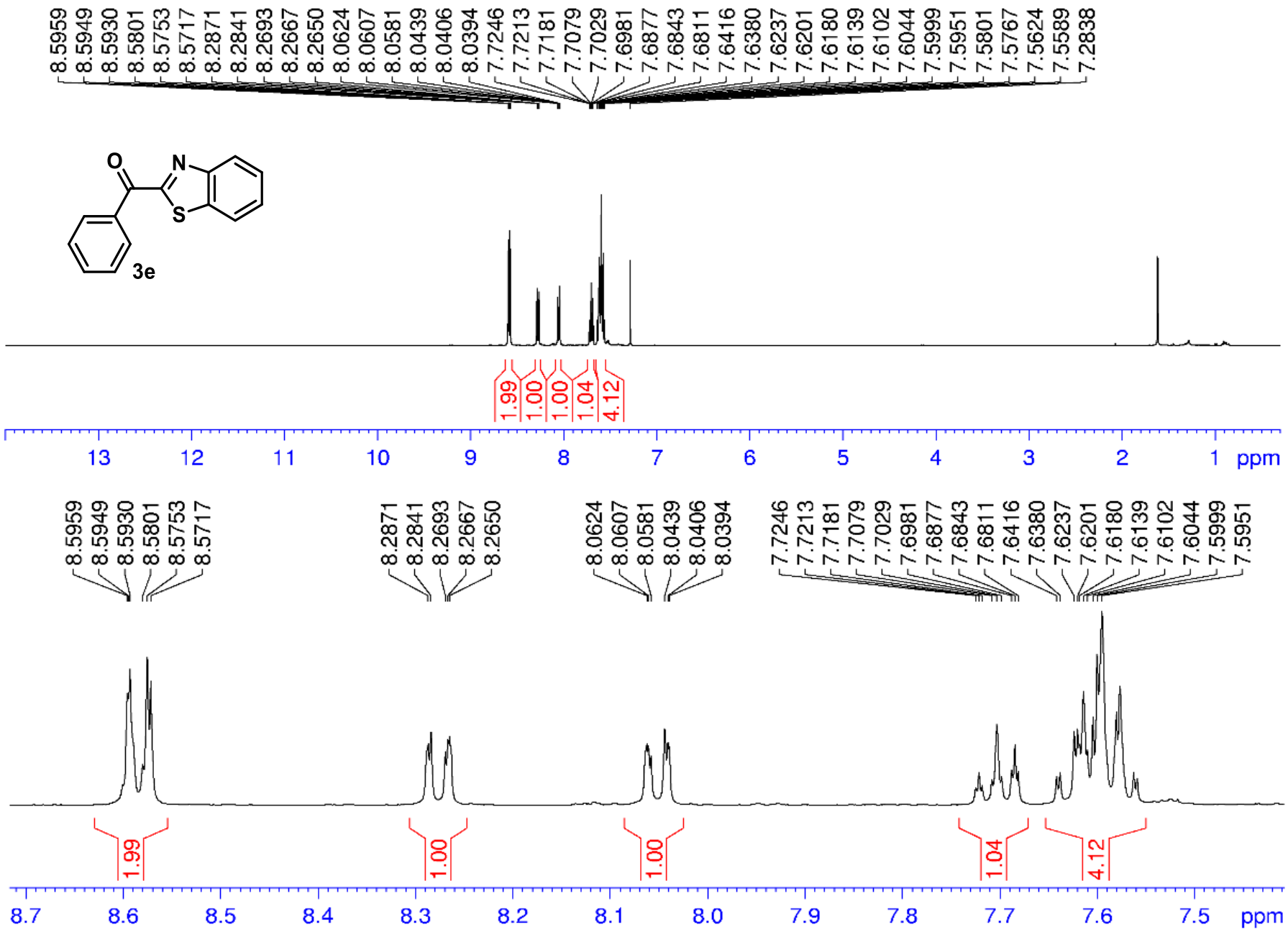
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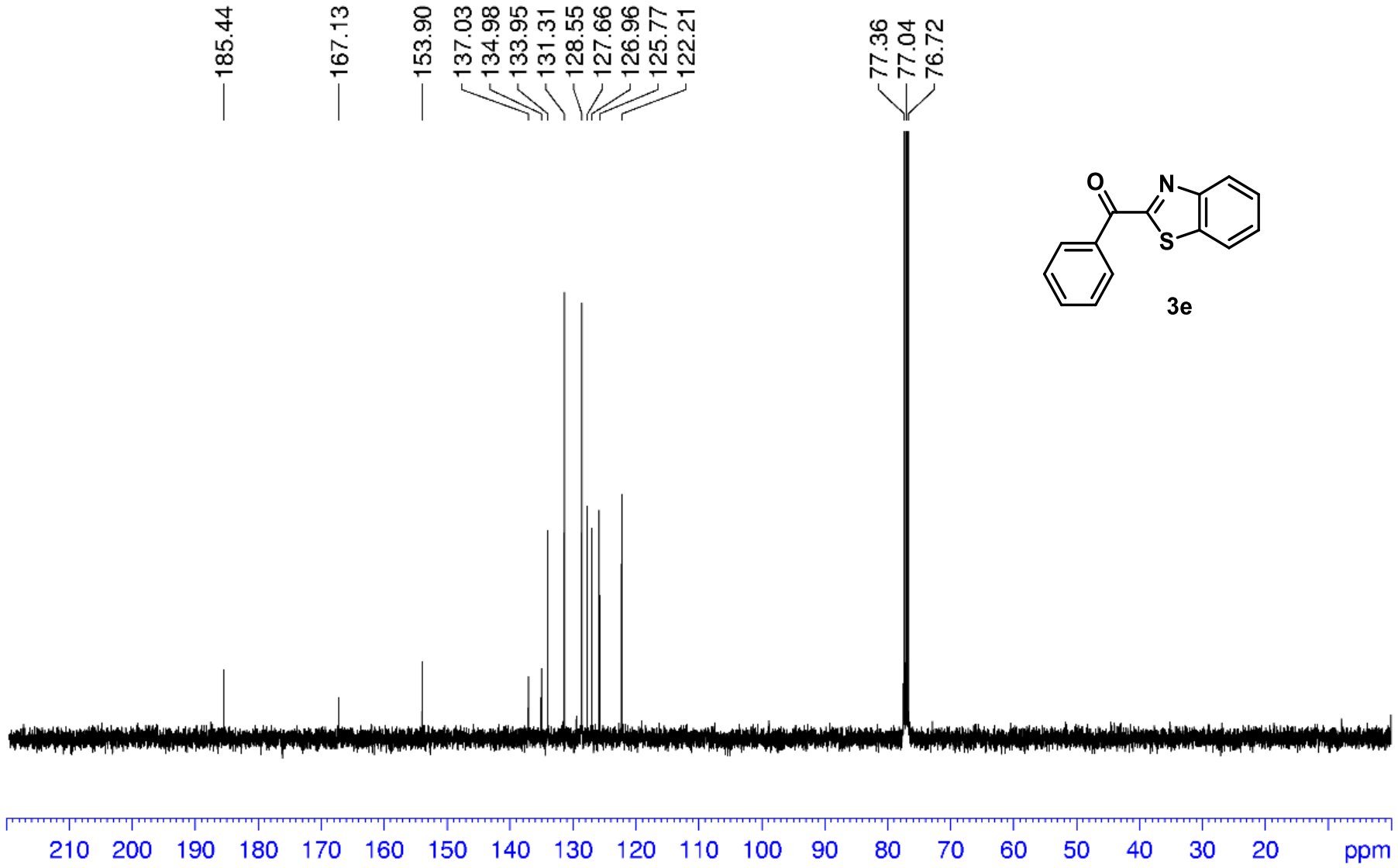
ppm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76.72
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N
S
3e
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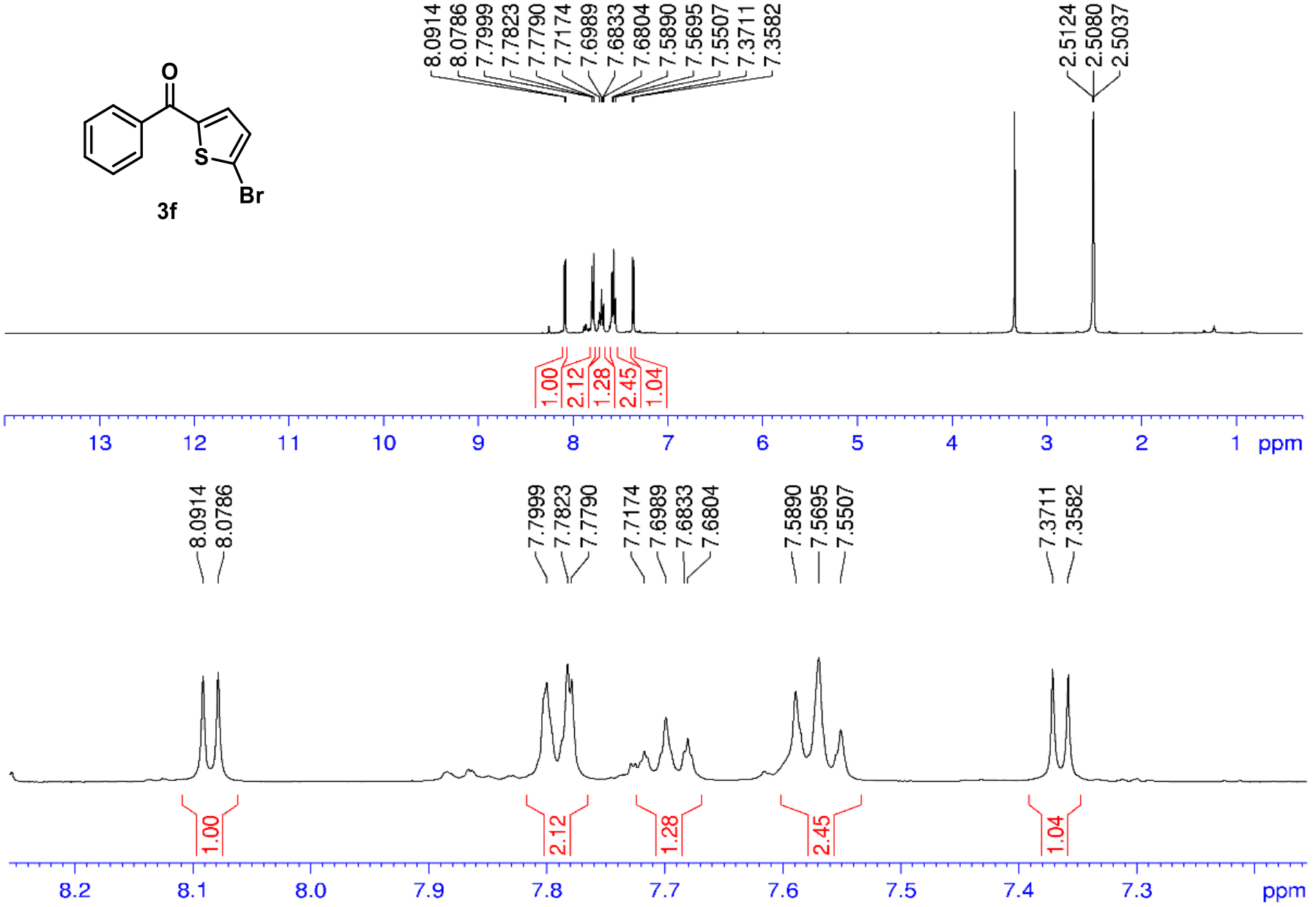
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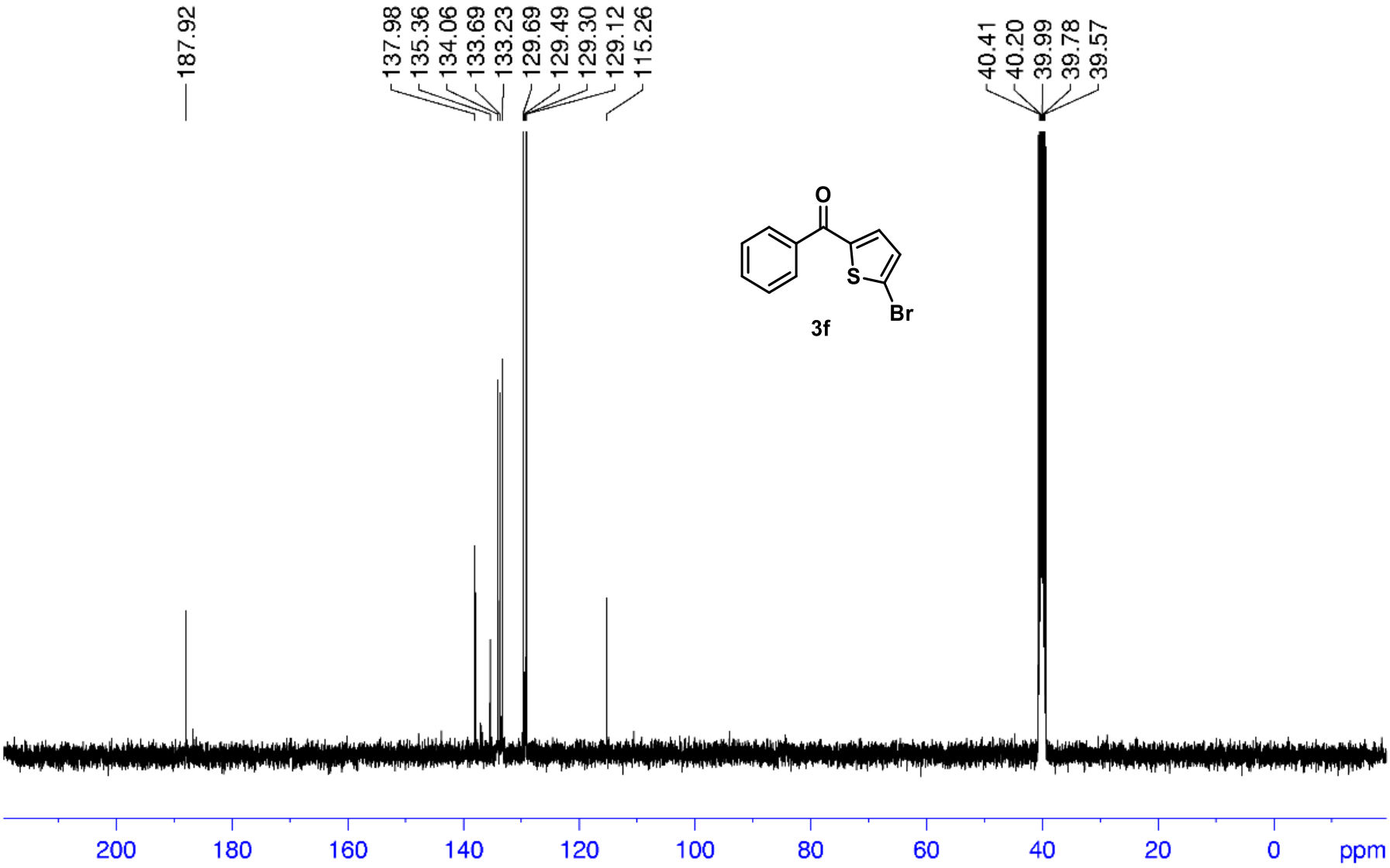
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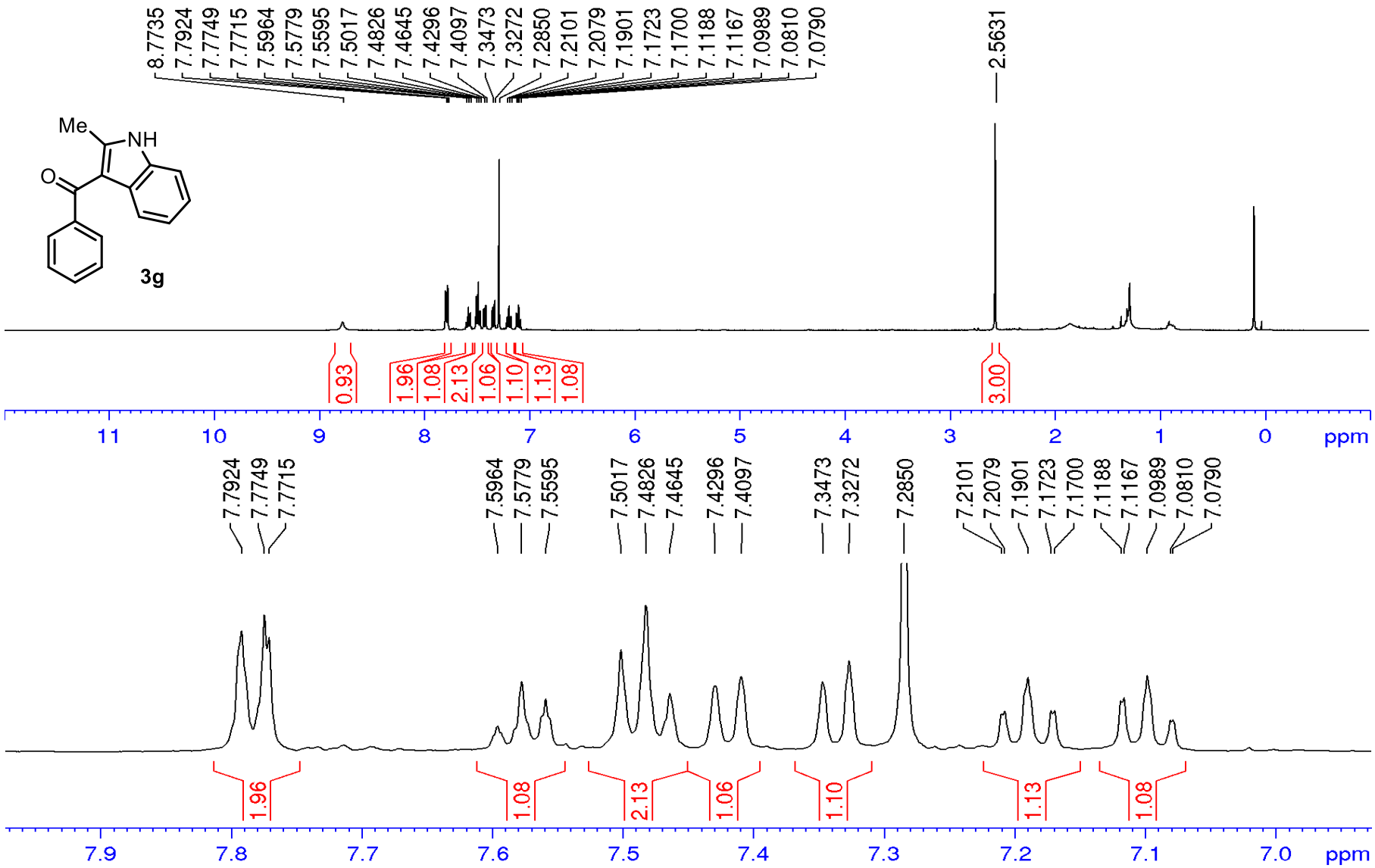
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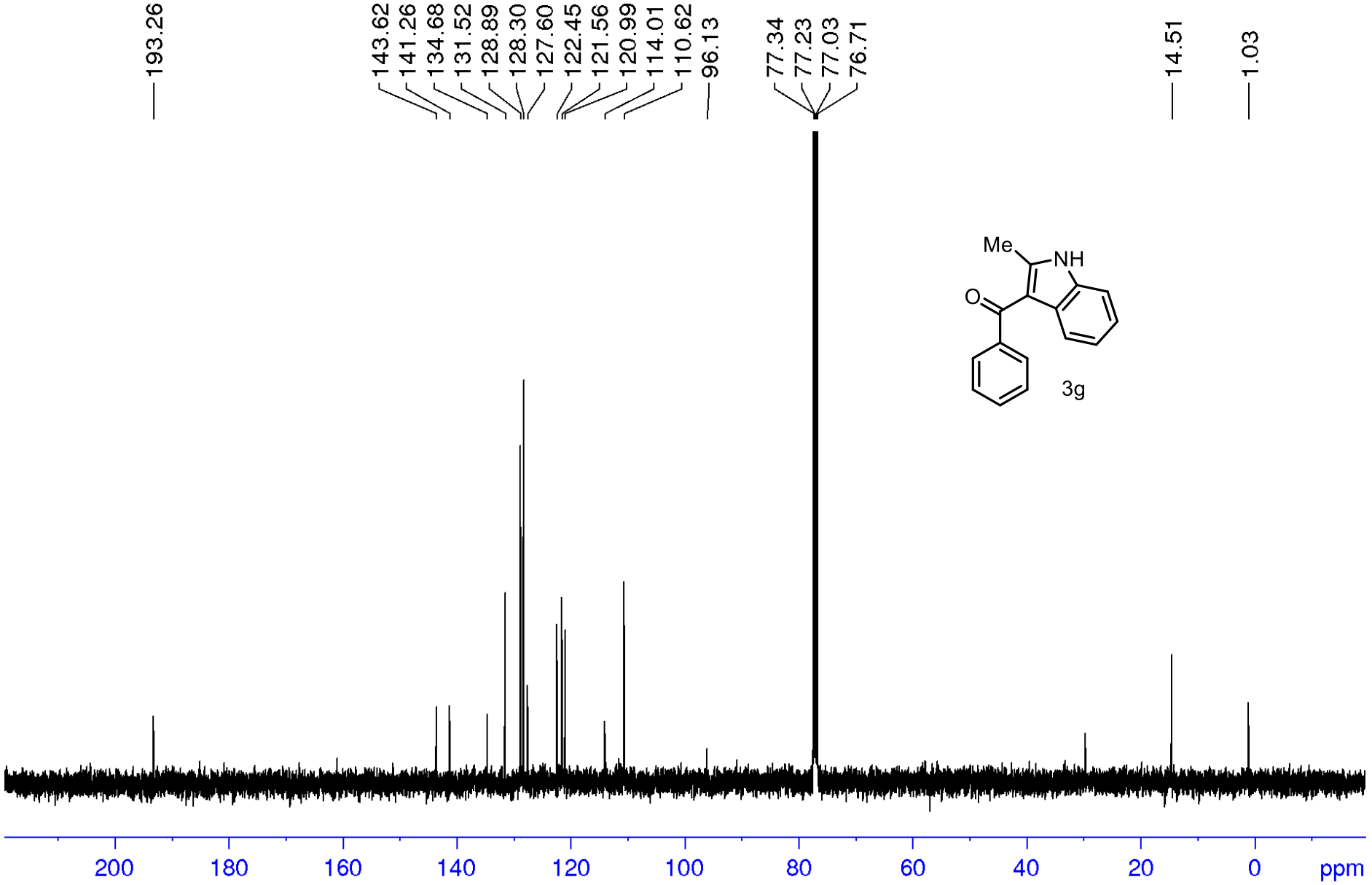
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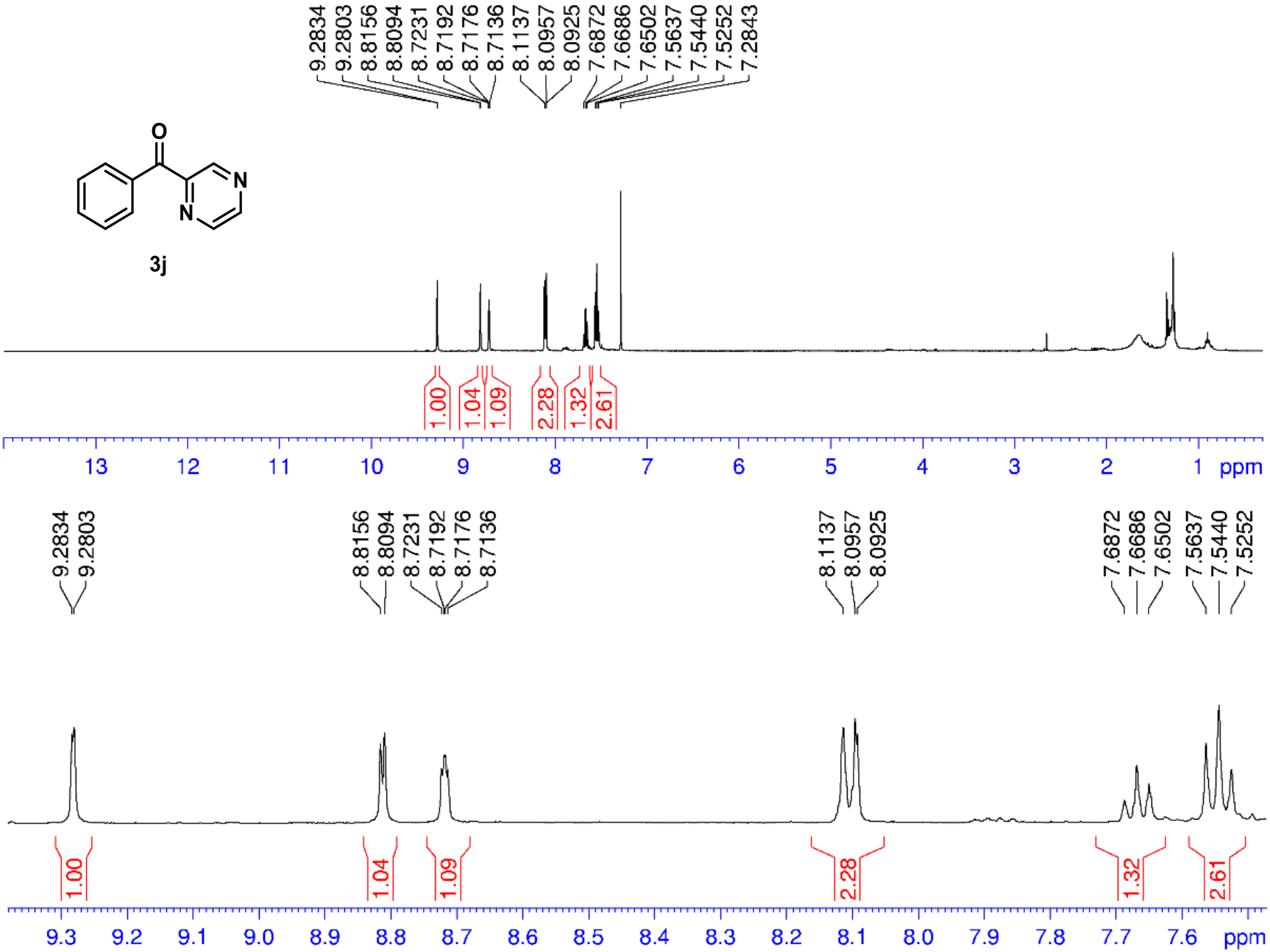
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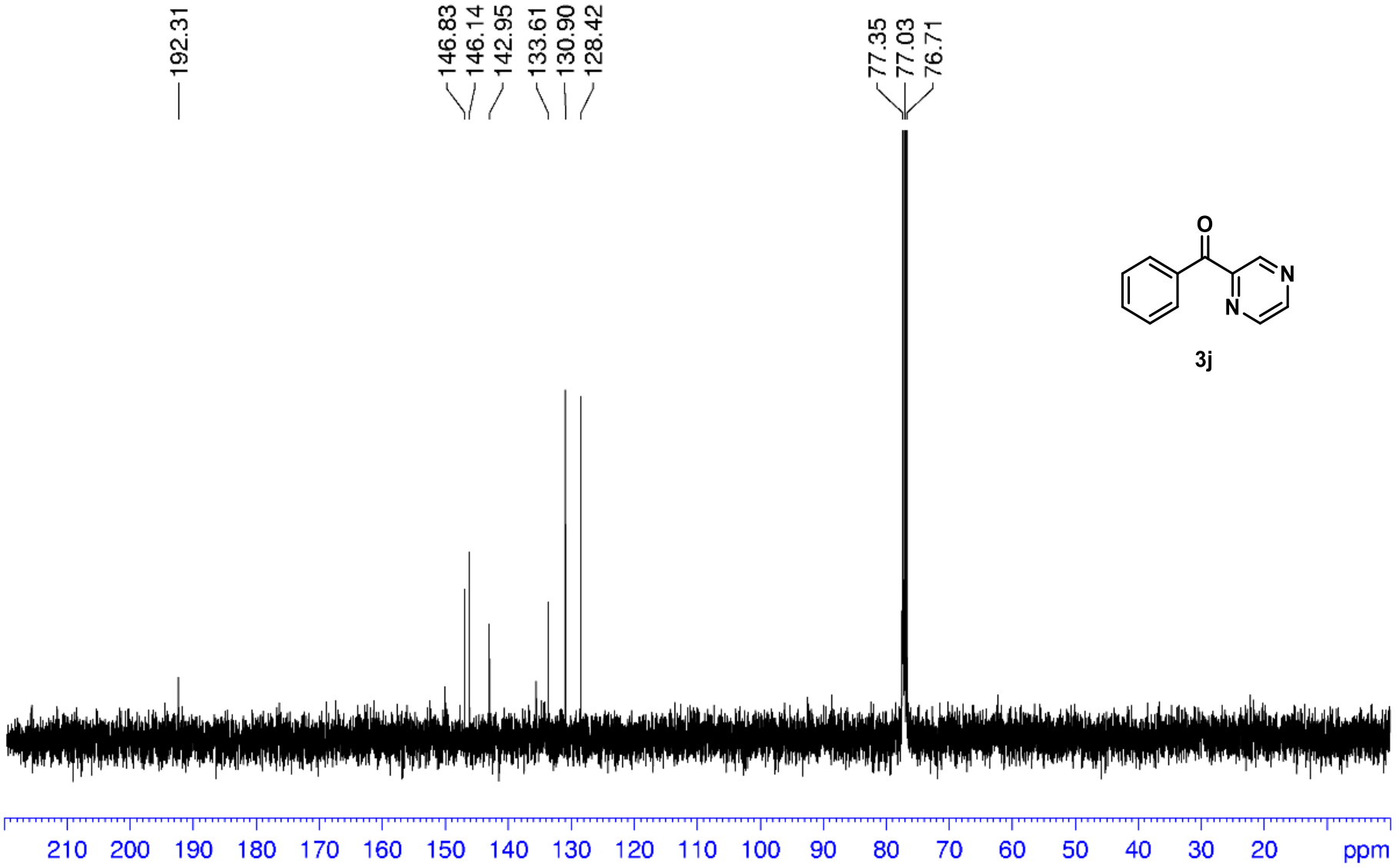
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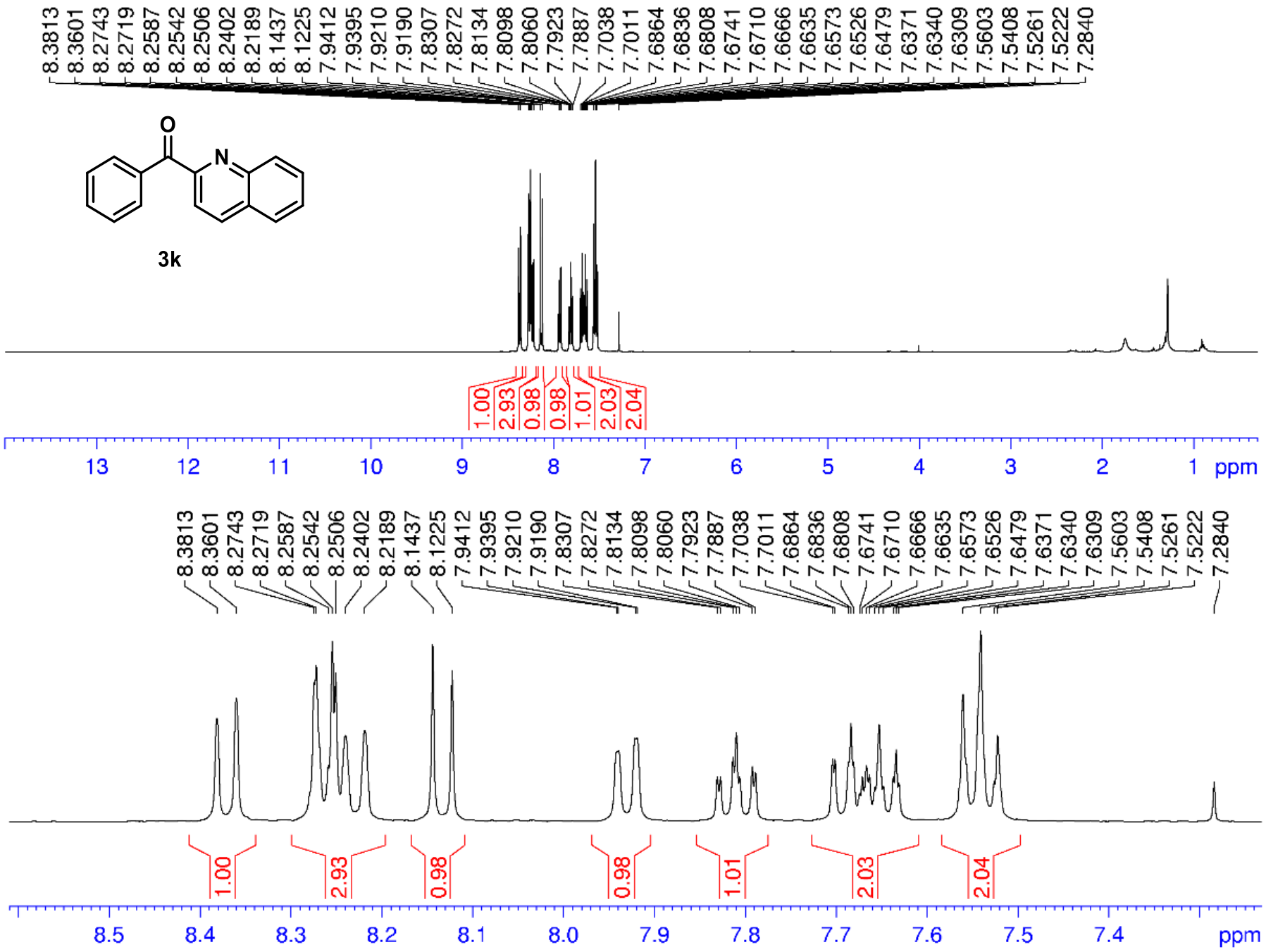
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7.6635
7.6573
7.6526
7.6479
7.6371
7.6340
7.6309
7.5603
7.5408
7.5261
7.5222
7.2840
O
N
3k
1.00
2.93
0.98
0.98
1.01
2.03
2.04
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
8.5
8.4
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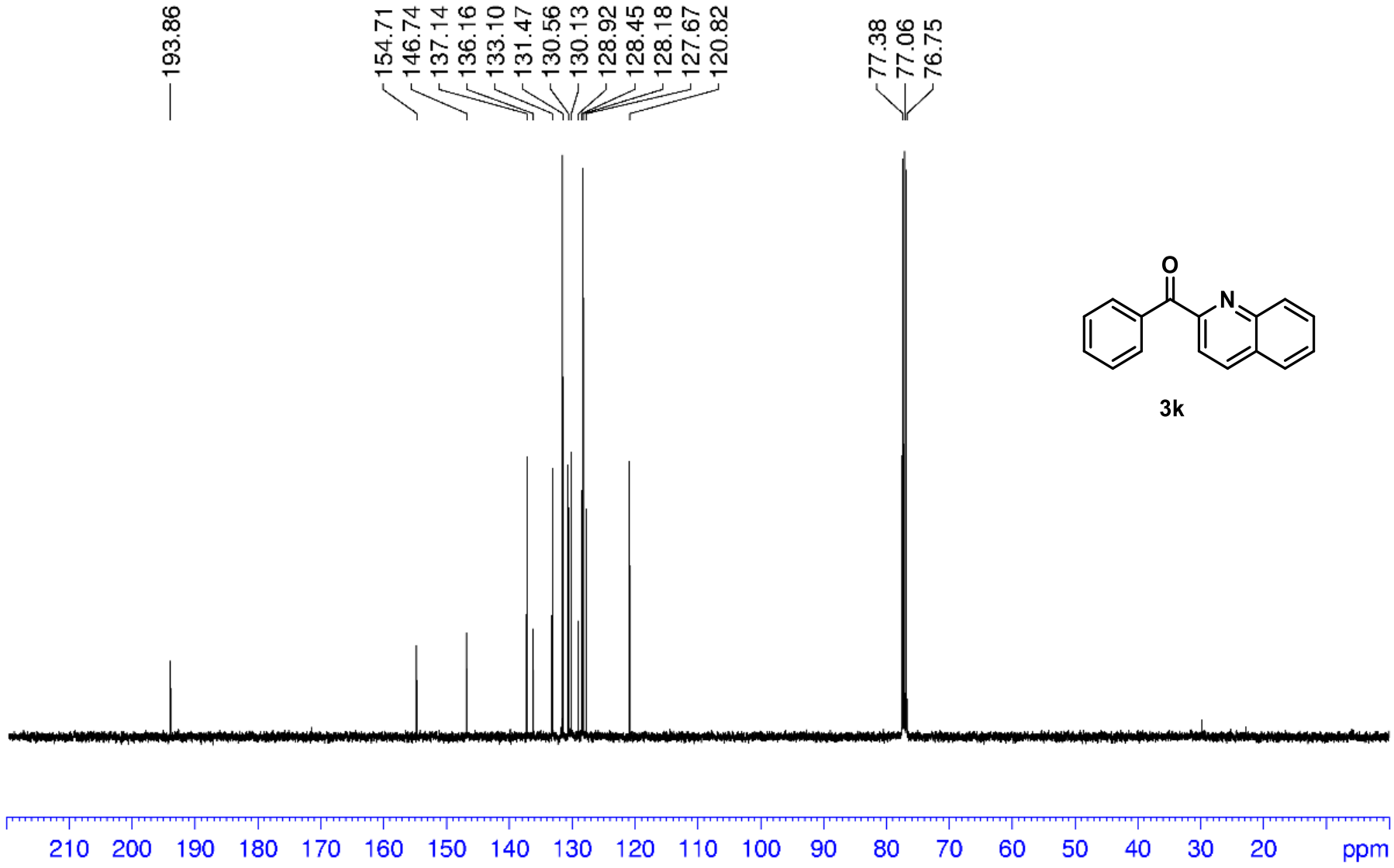
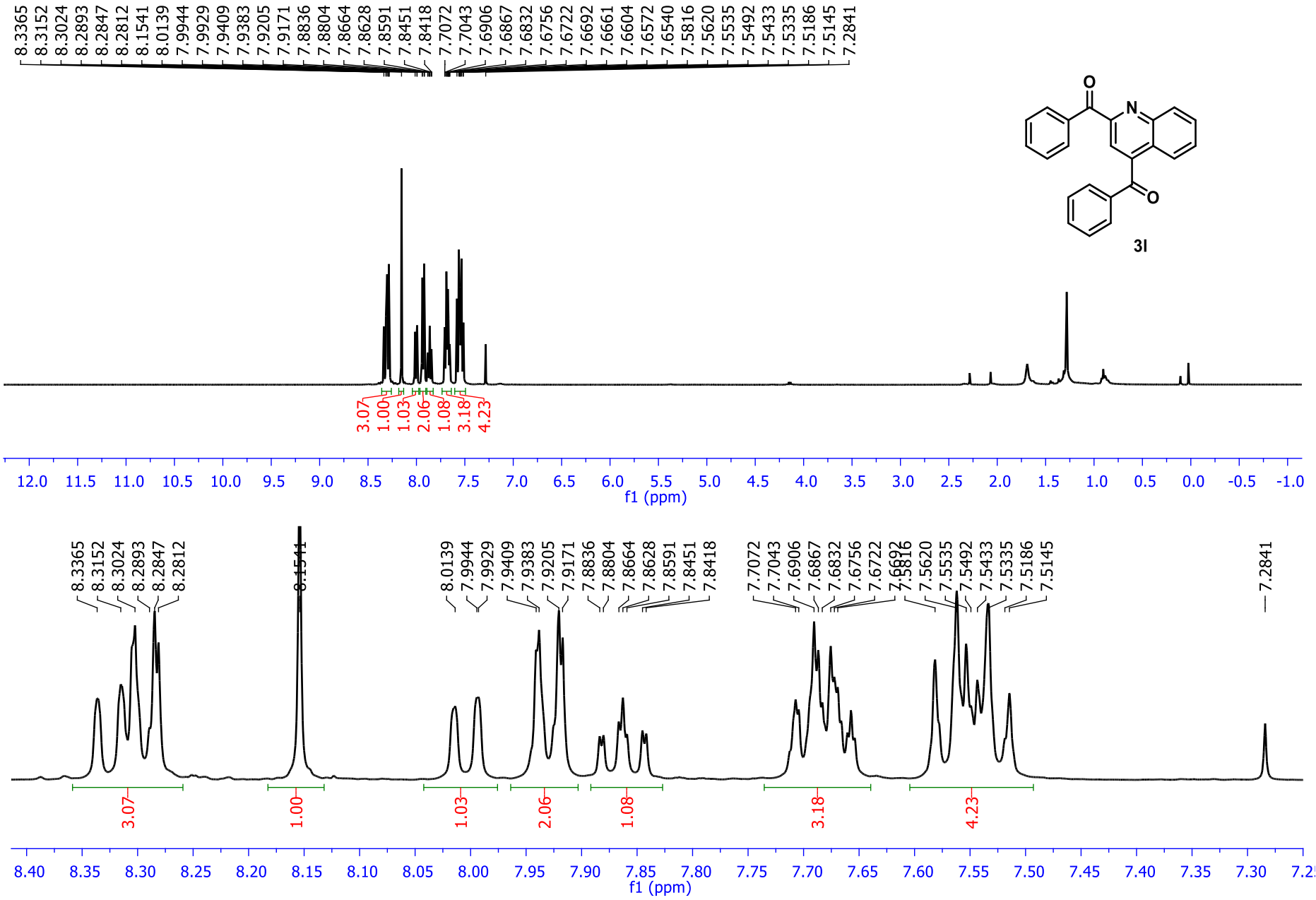
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm


193.86
154.71
146.74
137.14
136.16
133.10
131.47
130.56
130.13
128.92
128.45
128.18
127.67
120.82
77.38
77.06
76.75
O
N
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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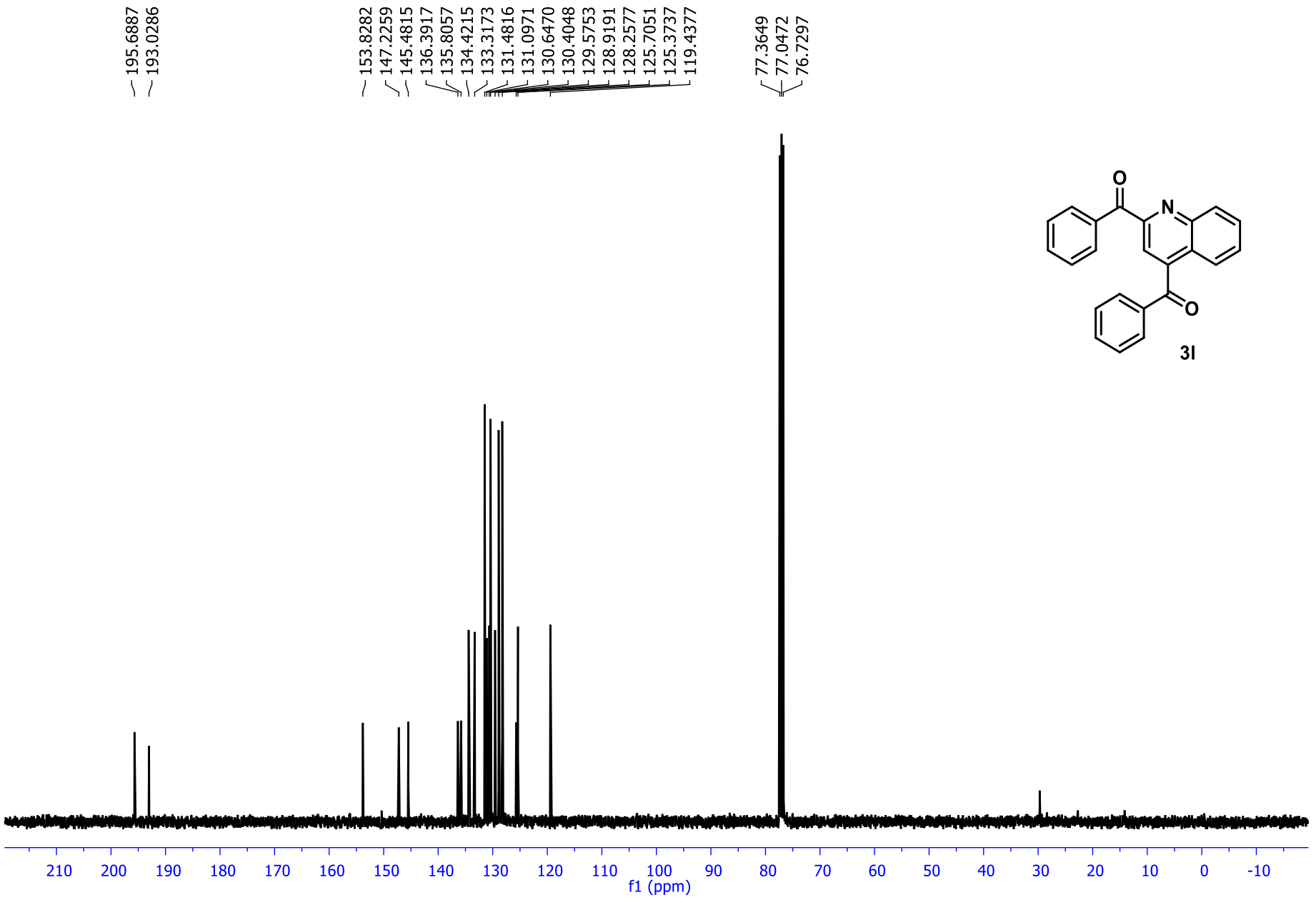
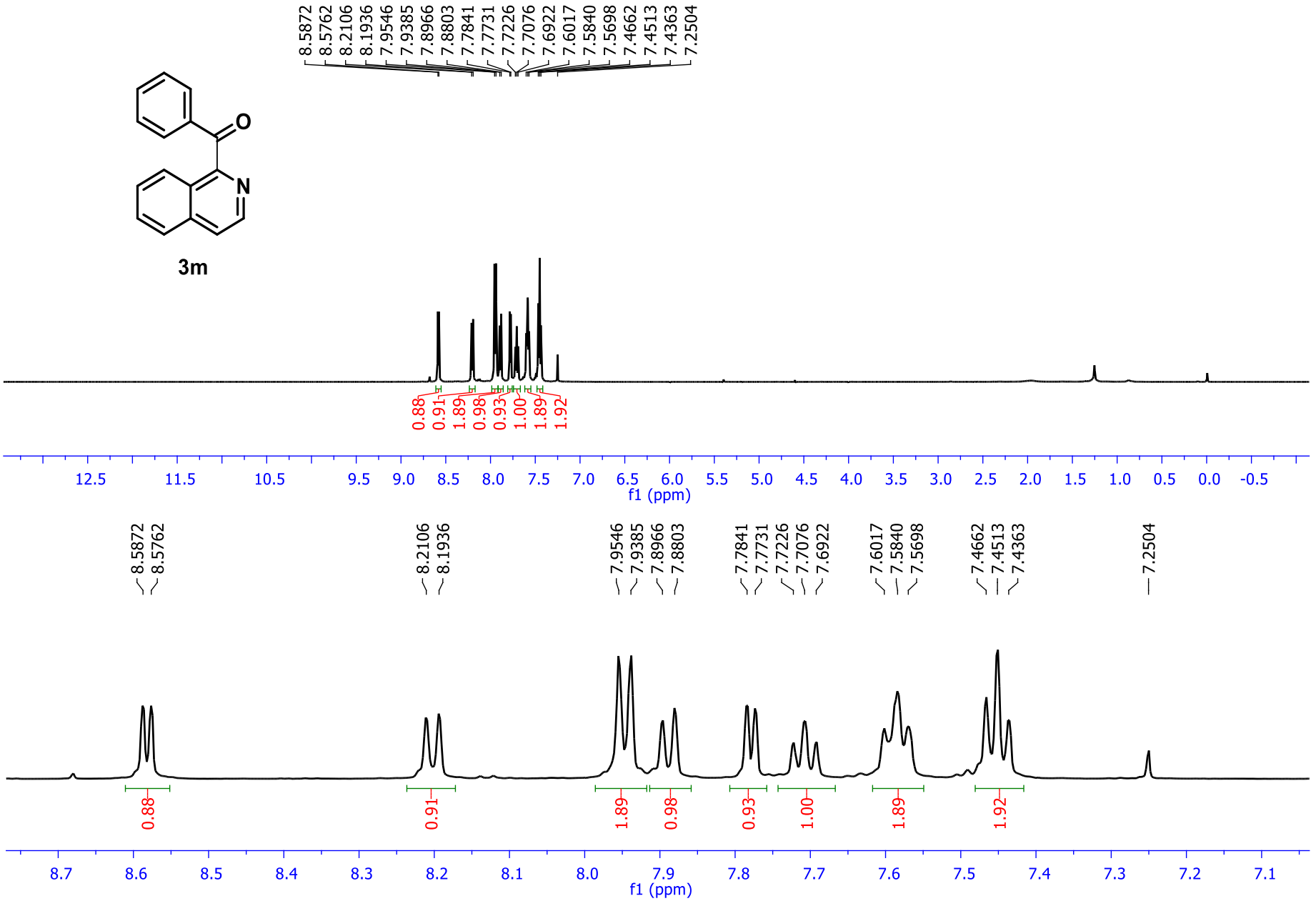
8.3152
8.3024
8.2893
8.2847
8.2812
8.1541
8.0139
7.9944
7.9929
7.9409
7.9383
7.9205
7.9171
7.8836
7.8804
7.8664
7.8628
7.8591
7.8451
7.8418
7.7072
7.7043
7.6906
7.6867
7.6832
7.6756
7.6722
7.6692
7.6661
7.6604
7.6572
7.6540
7.5816
7.5620
7.5535
7.5492
7.5433
7.5335
7.5186
7.5145
7.2841
O
N
O
3I
3.07
1.00
1.03
2.06
1.08
3.18
4.23
f1 (ppm)
f1 (ppm)


195.6887
193.0286
153.8282
147.2259
145.4815
136.3917
135.8057
134.4215
133.3173
131.4816
131.0971
130.6470
130.4048
129.5753
128.9191
128.2577
125.7051
125.3737
119.4377
77.3649
77.0472
76.7297
O
N
O
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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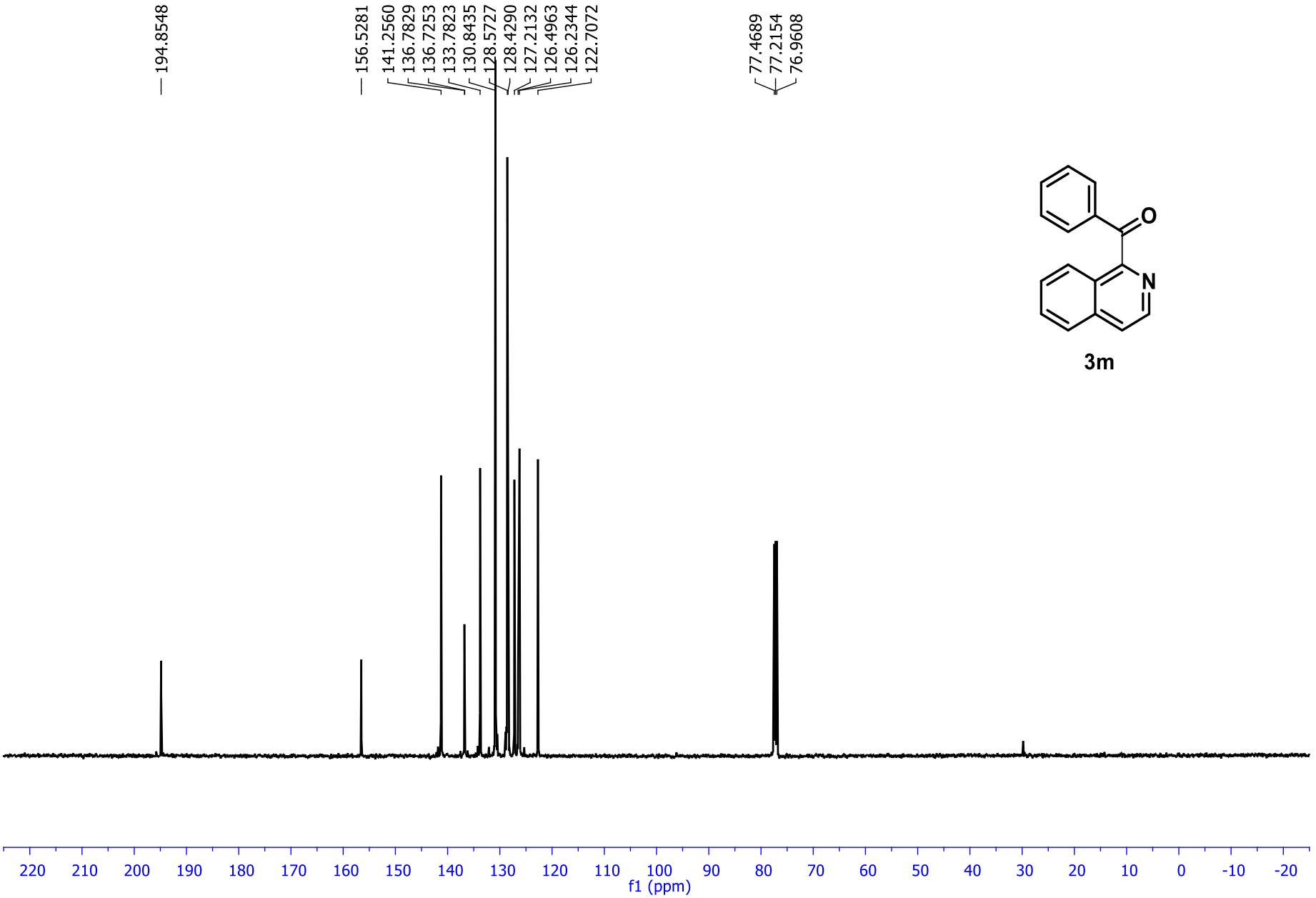
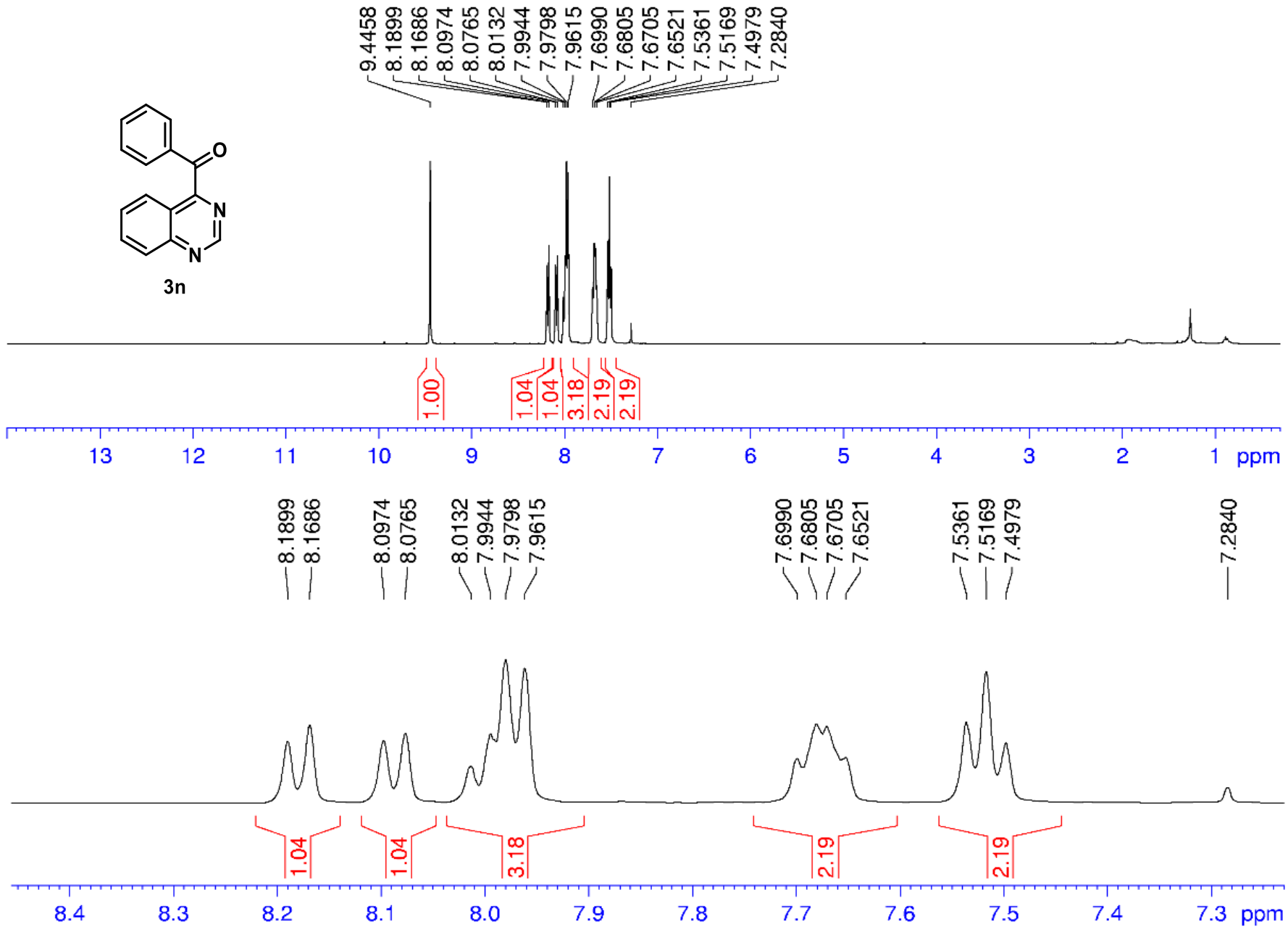
8.2106
8.1936
7.9546
7.9385
7.8966
7.8803
7.7841
7.7731
7.7226
7.7076
7.6922
7.6017
7.5840
7.5698
7.4662
7.4513
7.4363
7.2504
O
N
3m
0.88
0.91
1.89
0.98
0.93
1.00
1.89
1.92
f1 (ppm)


194.8548
156.5281
141.2560
136.7829
136.7253
133.7823
130.8435
128.5727
128.4290
127.2132
126.4963
126.2344
122.7072
77.4689
77.2154
76.9608
O
N
3m
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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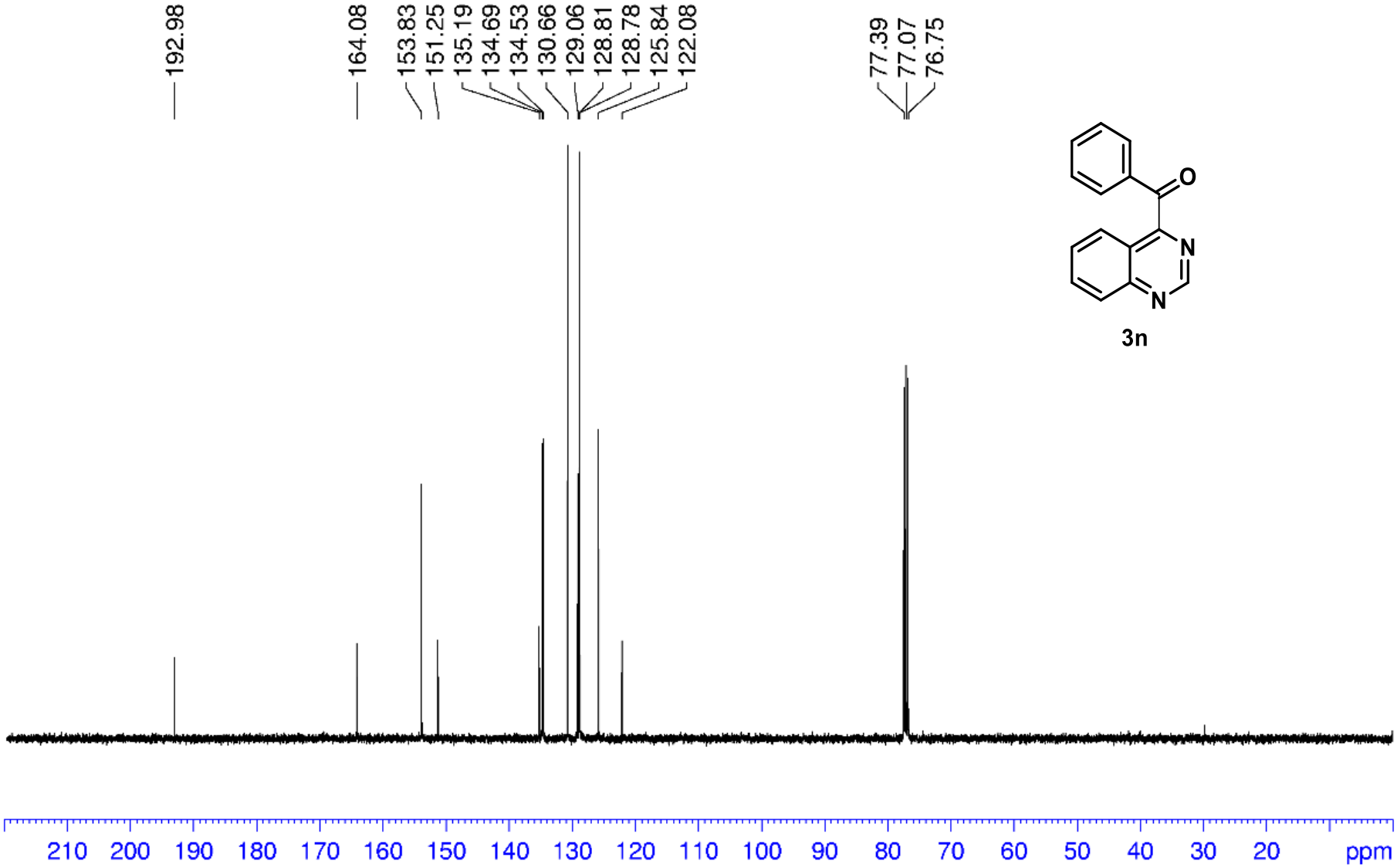
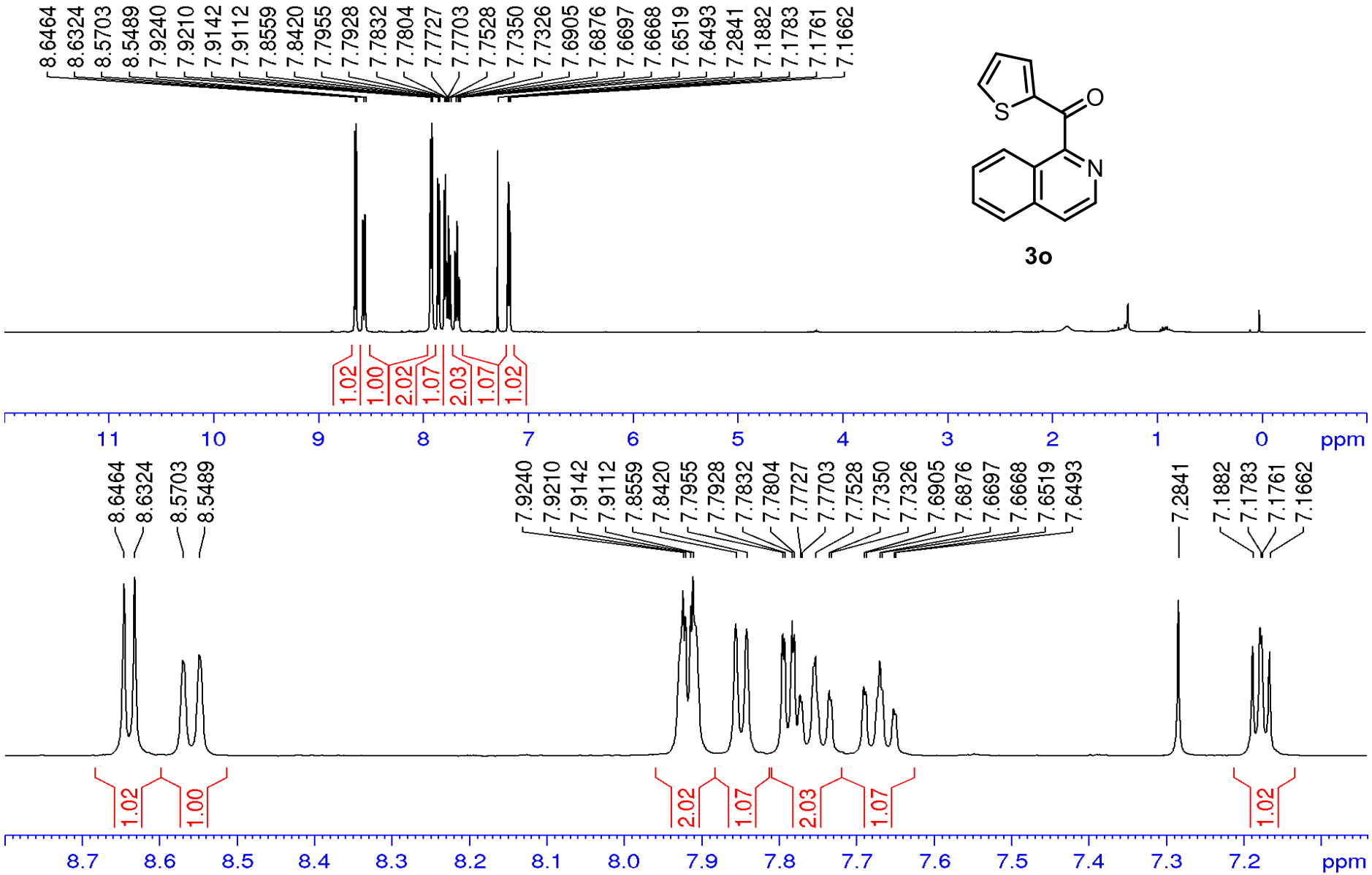
8.1899
8.1686
8.0974
8.0765
8.0132
7.9944
7.9798
7.9615
7.6990
7.6805
7.6705
7.6521
7.5361
7.5169
7.4979
7.2840
O
N
N
3n
1.00
1.04
1.04
3.18
2.19
2.19
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
8.1899
8.1686
8.0974
8.0765
8.0132
7.9944
7.9798
7.9615
7.6990
7.6805
7.6705
7.6521
7.5361
7.5169
7.4979
7.2840
1.04
1.04
3.18
2.19
2.19
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm


192.98
164.08
153.83
151.25
135.19
134.69
134.53
130.66
129.06
128.81
128.78
125.84
122.08
77.39
77.07
76.75
O
N
N
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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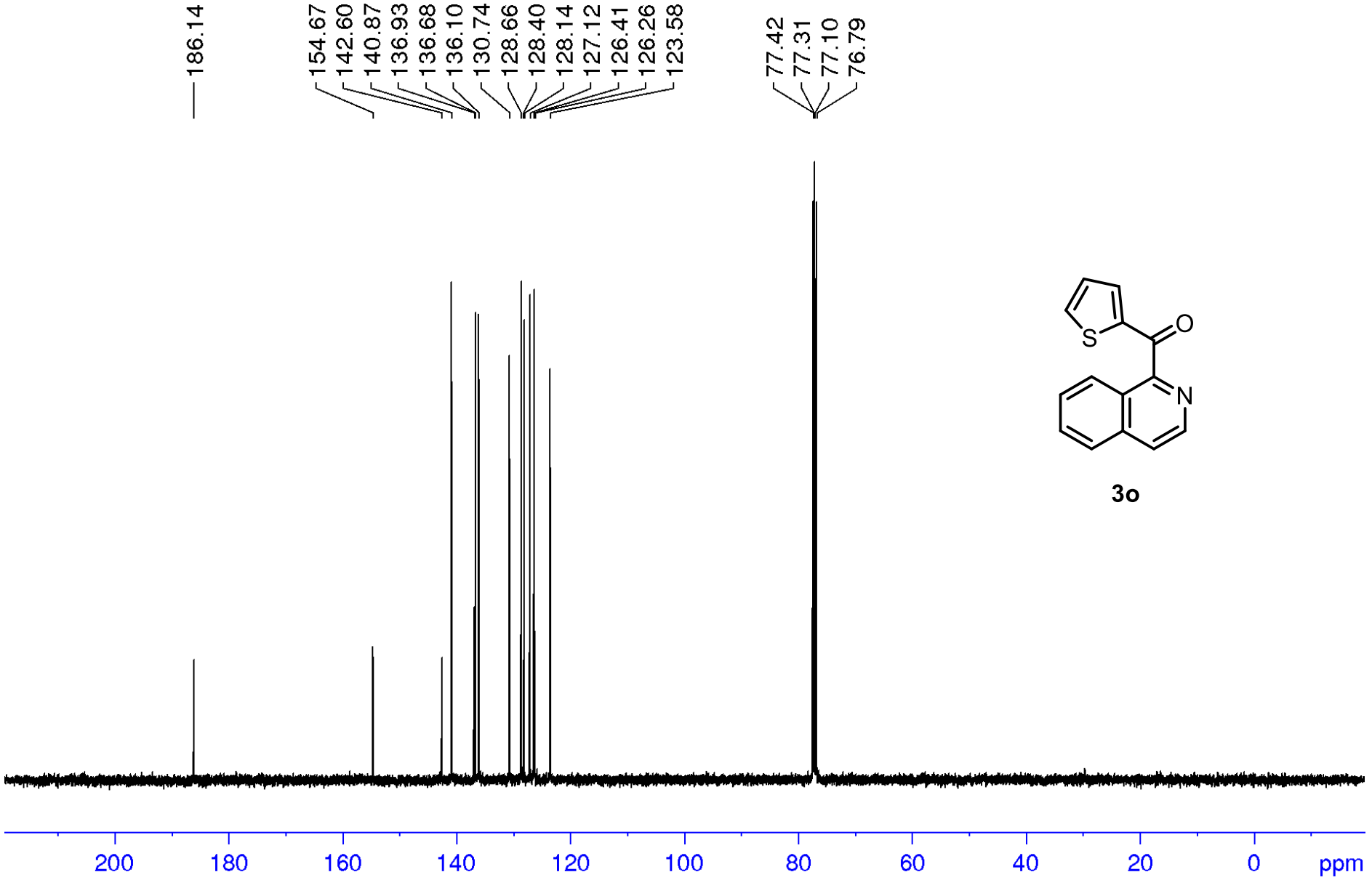
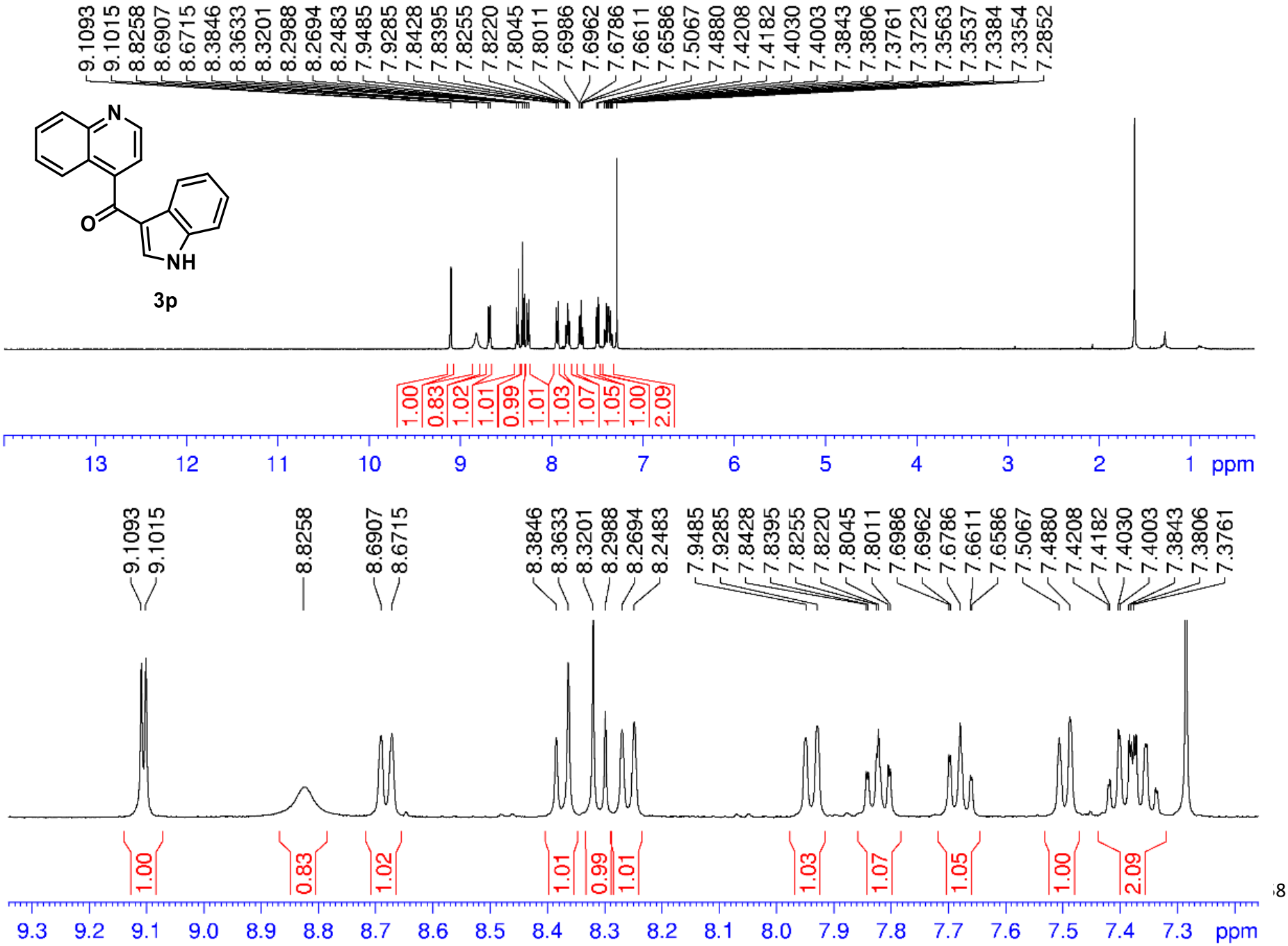
8.6324
8.5703
8.5489
7.9240
7.9210
7.9142
7.9112
7.8559
7.8420
7.7955
7.7928
7.7832
7.7804
7.7727
7.7703
7.7528
7.7350
7.7326
7.6905
7.6876
7.6697
7.6668
7.6519
7.6493
7.2841
7.1882
7.1783
7.1761
7.1662
S
O
N
3o
1.02
1.00
2.02
1.07
2.03
1.07
1.02
11
10
9
8
7
6
5
4
3
2
1
0
ppm
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm


186.14
154.67
142.60
140.87
136.93
136.68
136.10
130.74
128.66
128.40
128.14
127.12
126.41
126.26
123.58
77.42
77.31
77.10
76.79
S
O
N
200
180
160
140
120
100
80
60
40
20
0
ppm

**3o**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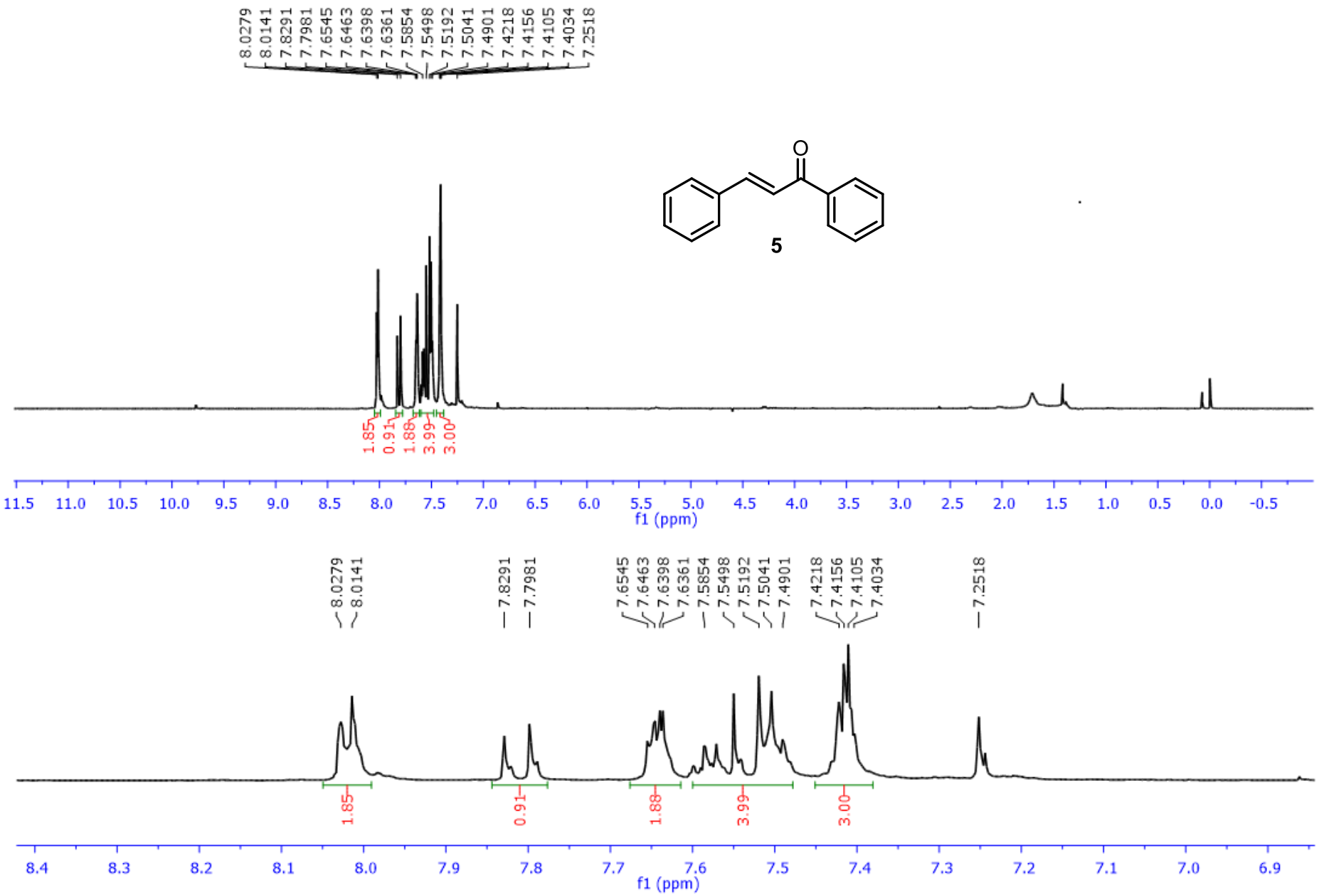
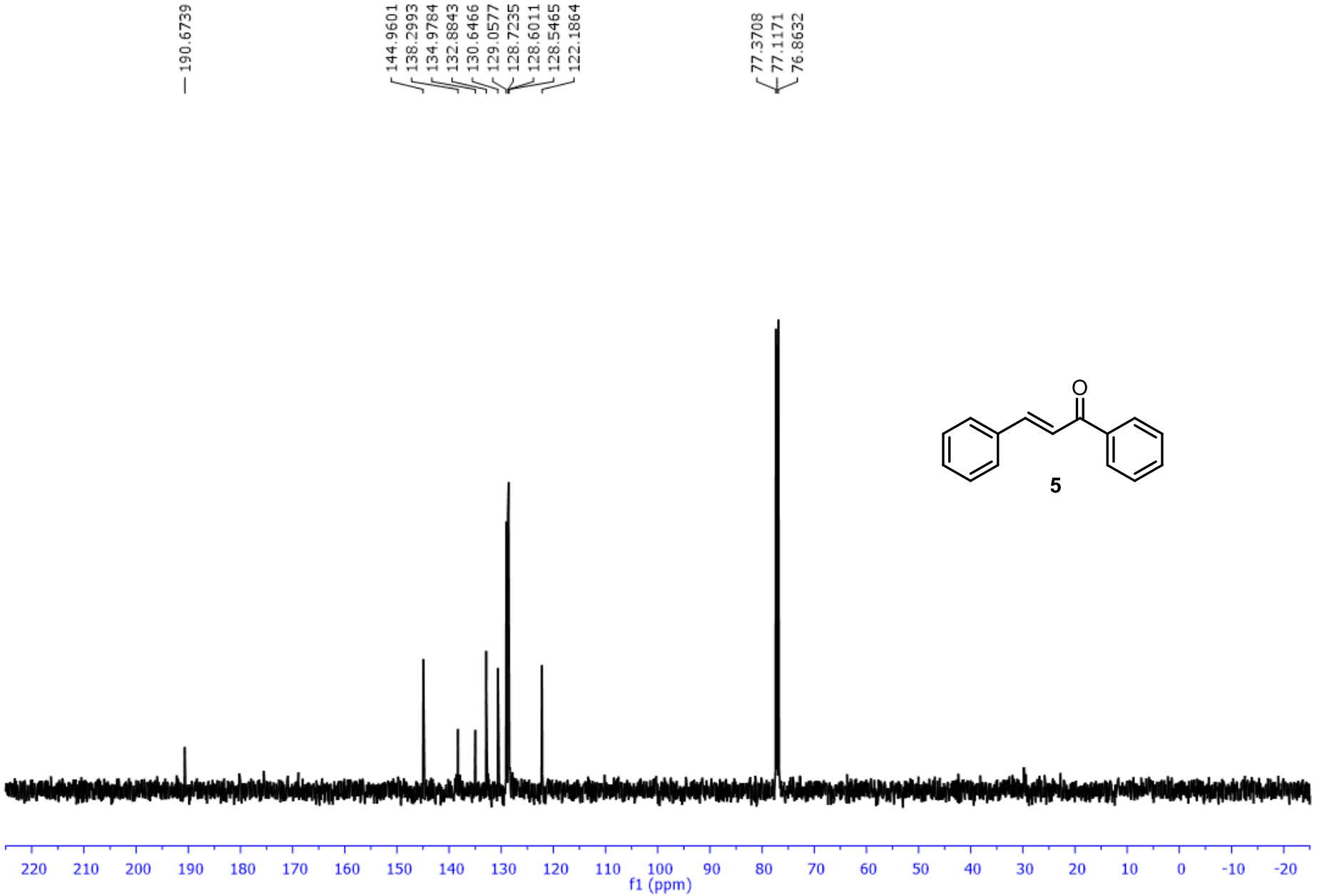
9.1015
8.8258
8.6907
8.6715
8.3846
8.3633
8.3201
8.2988
8.2694
8.2483
7.9485
7.9285
7.8428
7.8395
7.8255
7.8220
7.8045
7.8011
7.6986
7.6962
7.6786
7.6611
7.6586
7.5067
7.4880
7.4208
7.4182
7.4030
7.4003
7.3843
7.3806
7.3761
7.3723
7.3563
7.3537
7.3384
7.3354
7.2852
N
O
NH
3p
1.00
0.83
1.02
1.01
0.99
1.01
1.03
1.07
1.05
1.00
2.09
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm


8.0279
8.0141
7.8291
7.7981
7.6545
7.6463
7.6398
7.6361
7.5854
7.5498
7.5192
7.5041
7.4901
7.4218
7.4156
7.4105
7.4034
7.2518
O
5
1.85
0.91
1.88
3.99
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)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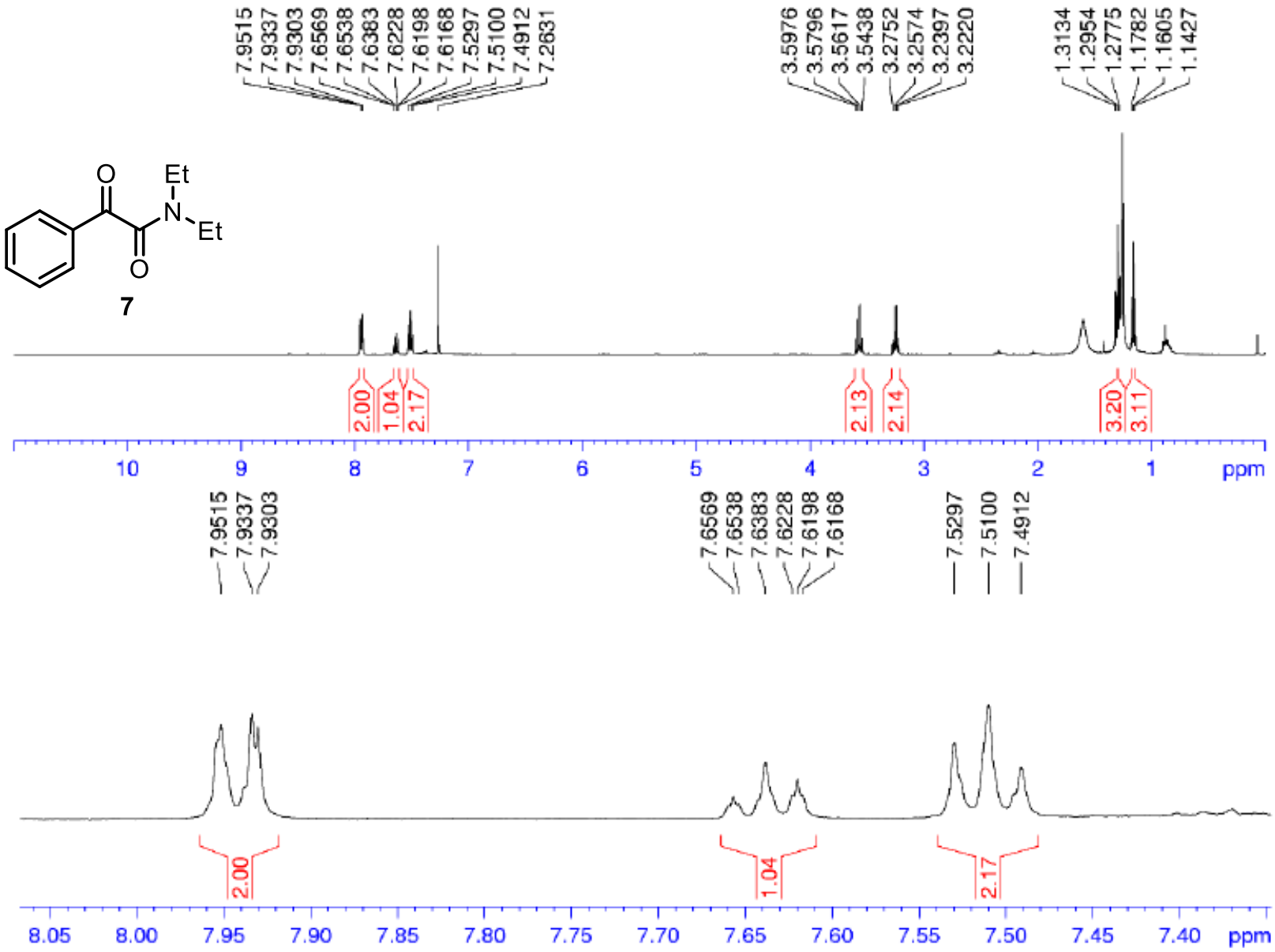
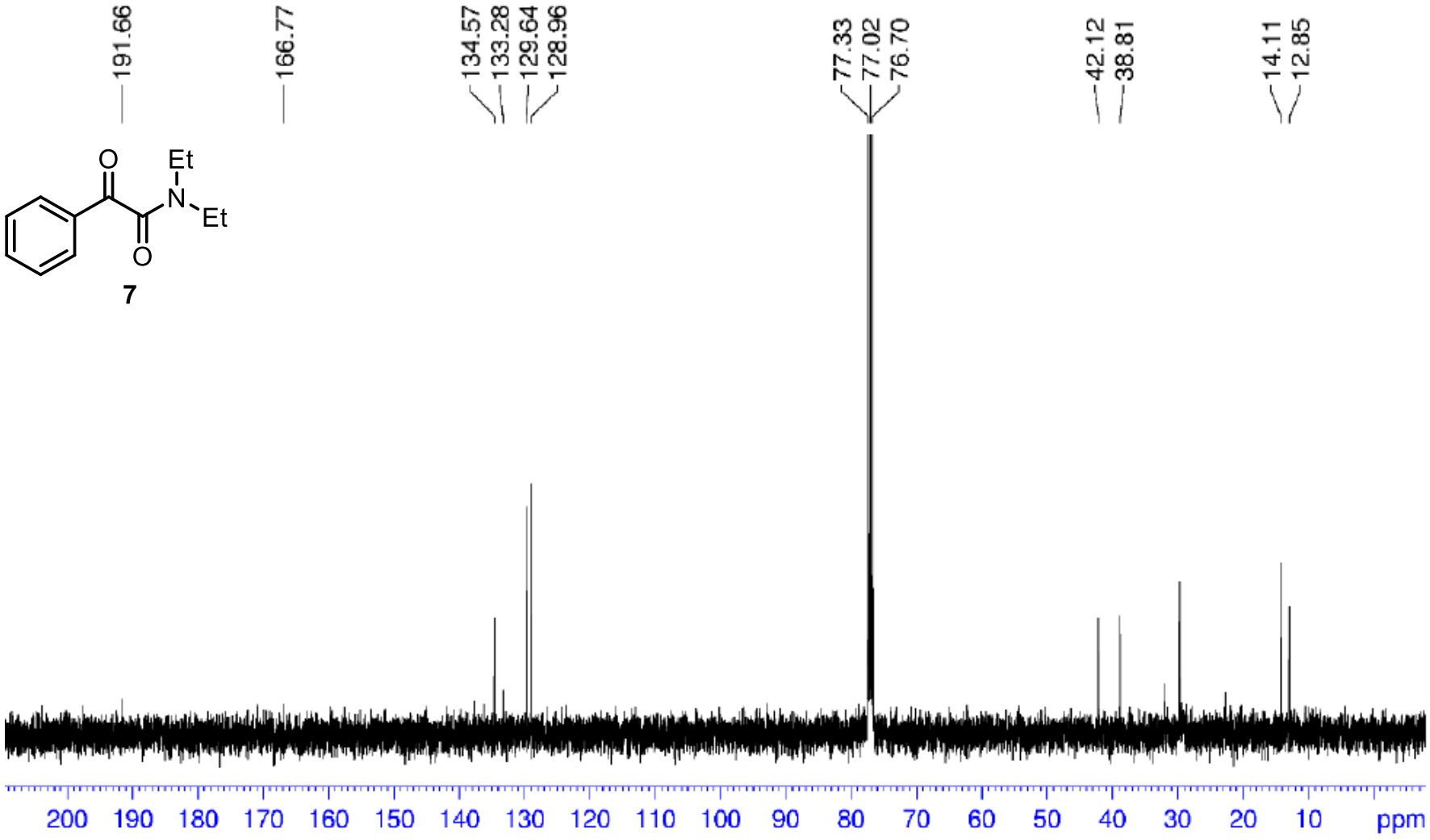
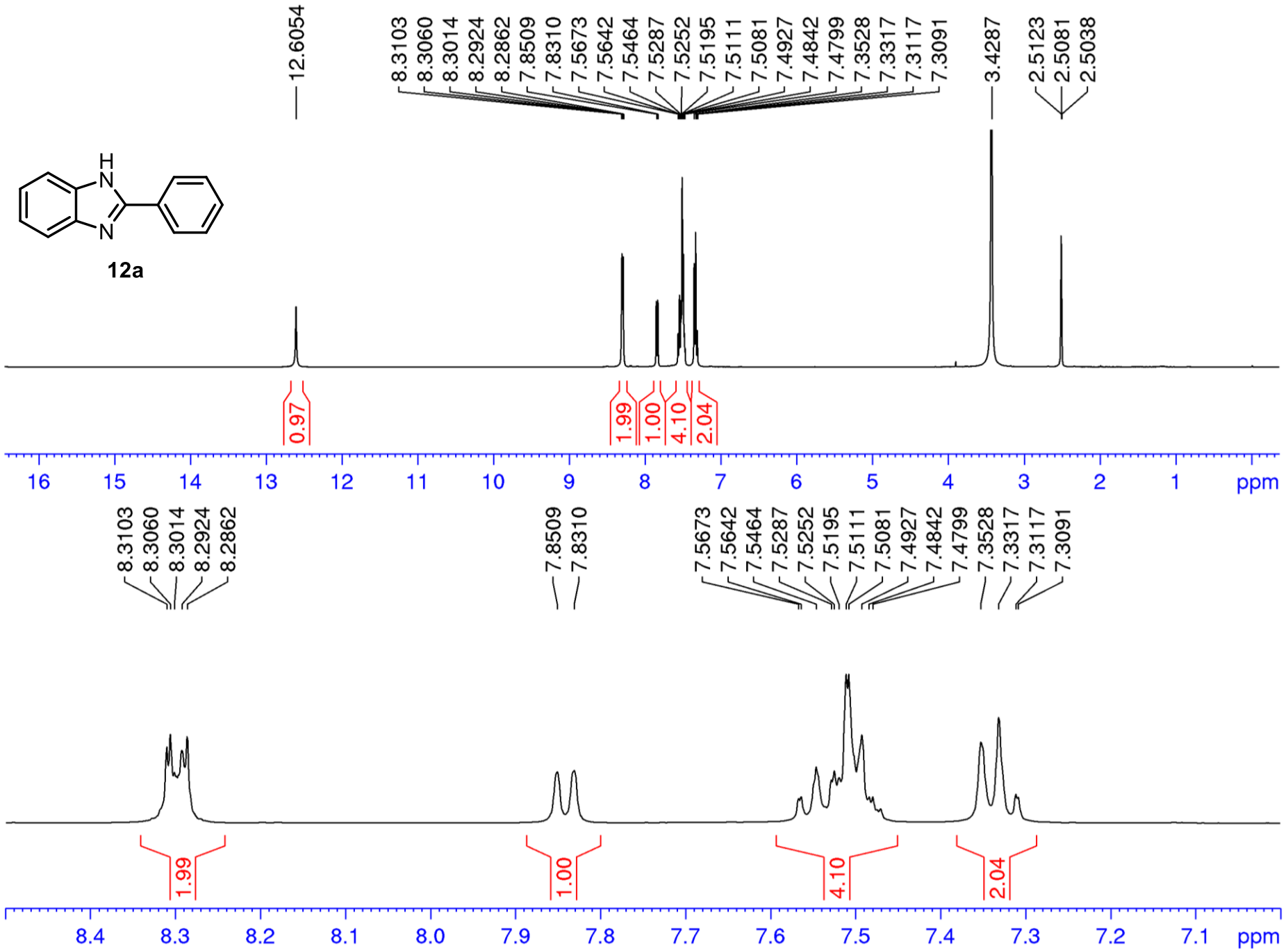
144.9601
138.2993
134.9784
132.8843
130.6466
129.0577
128.7235
128.6011
128.5465
122.1864
77.3708
77.1171
76.8632
O
5
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


7.9515
7.9337
7.9303
7.6569
7.6538
7.6383
7.6228
7.6198
7.6168
7.5297
7.5100
7.4912
7.2631
3.5976
3.5796
3.5617
3.5438
3.2752
3.2574
3.2397
3.2220
1.3134
1.2954
1.2775
1.1782
1.1605
1.1427
O
Et
N
Et
O
7
2.00
1.04
2.17
2.13
2.14
3.20
3.11
10
9
8
7
6
5
4
3
2
1
ppm
7.9515
7.9337
7.9303
7.6569
7.6538
7.6383
7.6228
7.6198
7.6168
7.5297
7.5100
7.4912
2.00
1.04
2.17
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
ppm


191.66
166.77
134.57
133.28
129.64
128.96
77.33
77.02
76.70
42.12
38.81
14.11
12.85
O
Et
N
Et
O
7
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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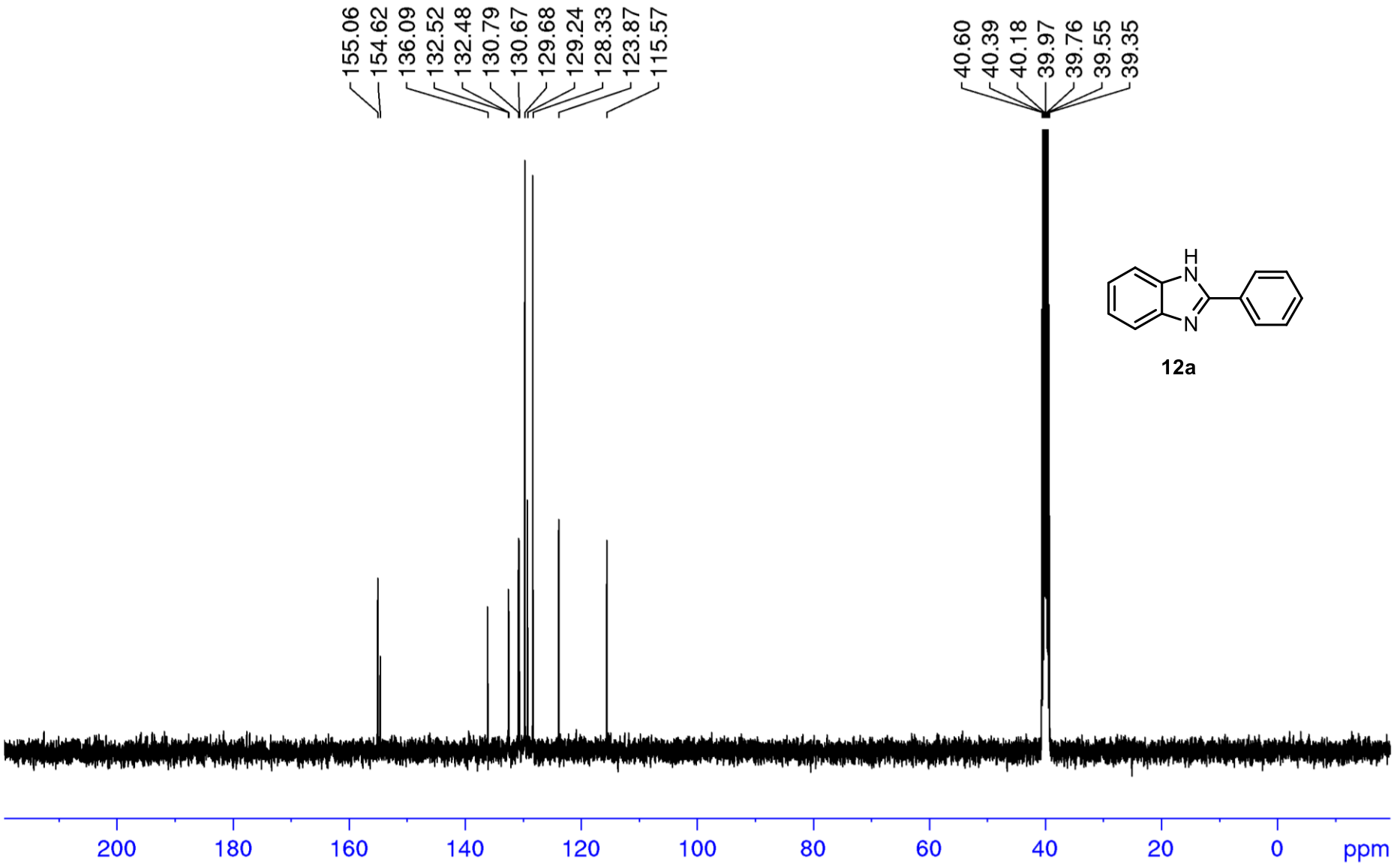
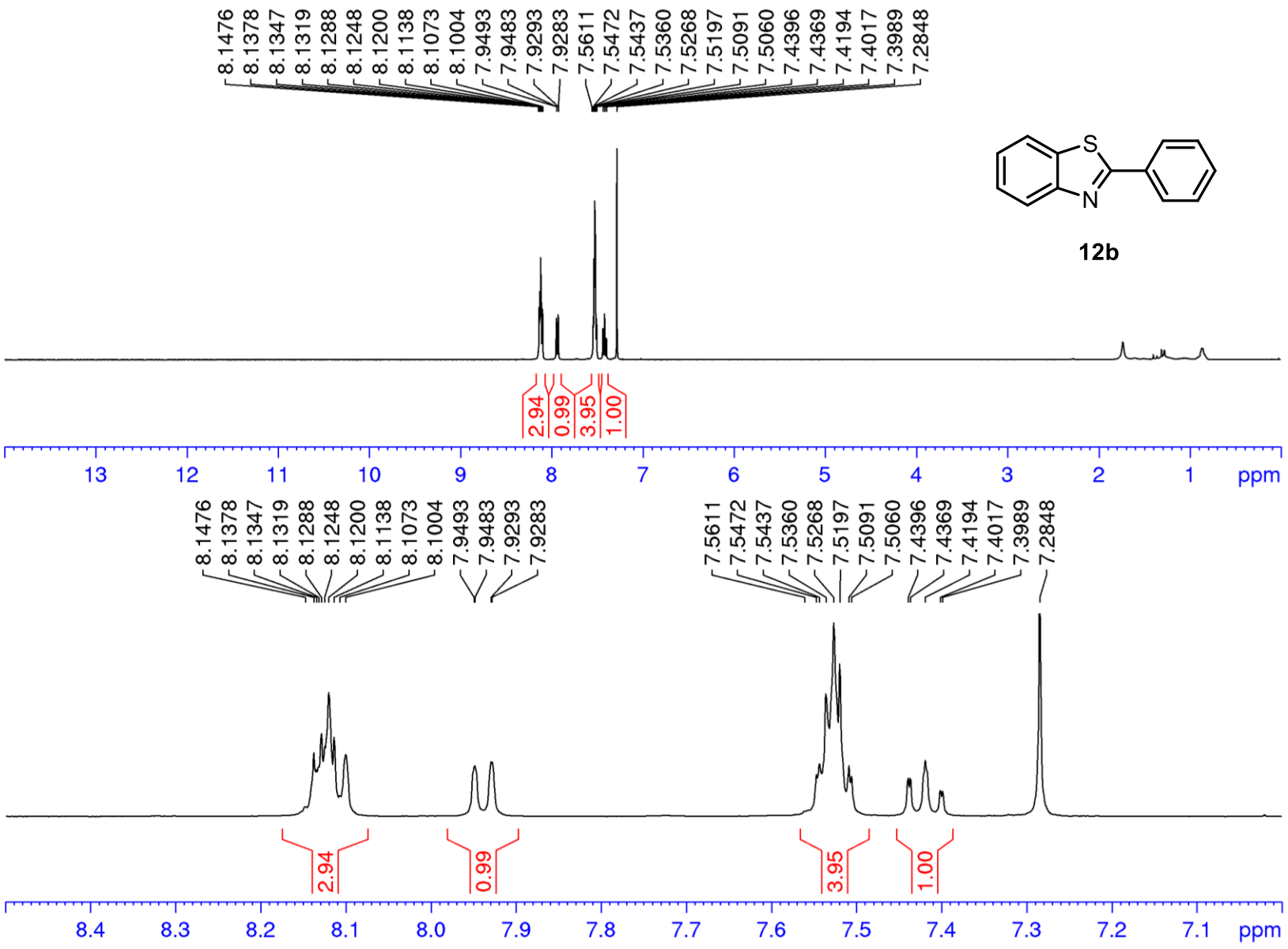
8.3103
8.3060
8.3014
8.2924
8.2862
7.8509
7.8310
7.5673
7.5642
7.5464
7.5287
7.5252
7.5195
7.5111
7.5081
7.4927
7.4842
7.4799
7.3528
7.3317
7.3117
7.3091
3.4287
2.5123
2.5081
2.5038
H
N
N
12a
0.97
1.99
1.00
4.10
2.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
8.3103
8.3060
8.3014
8.2924
8.2862
7.8509
7.8310
7.5673
7.5642
7.5464
7.5287
7.5252
7.5195
7.5111
7.5081
7.4927
7.4842
7.4799
7.3528
7.3317
7.3117
7.3091
1.99
1.00
4.10
2.04
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm


155.06
154.62
136.09
132.52
132.48
130.79
130.67
129.68
129.24
128.33
123.87
115.57
40.60
40.39
40.18
39.97
39.76
39.55
39.35
H
N
N
12a
200
180
160
140
120
100
80
60
40
20
0
ppm


8.1476
8.1378
8.1347
8.1319
8.1288
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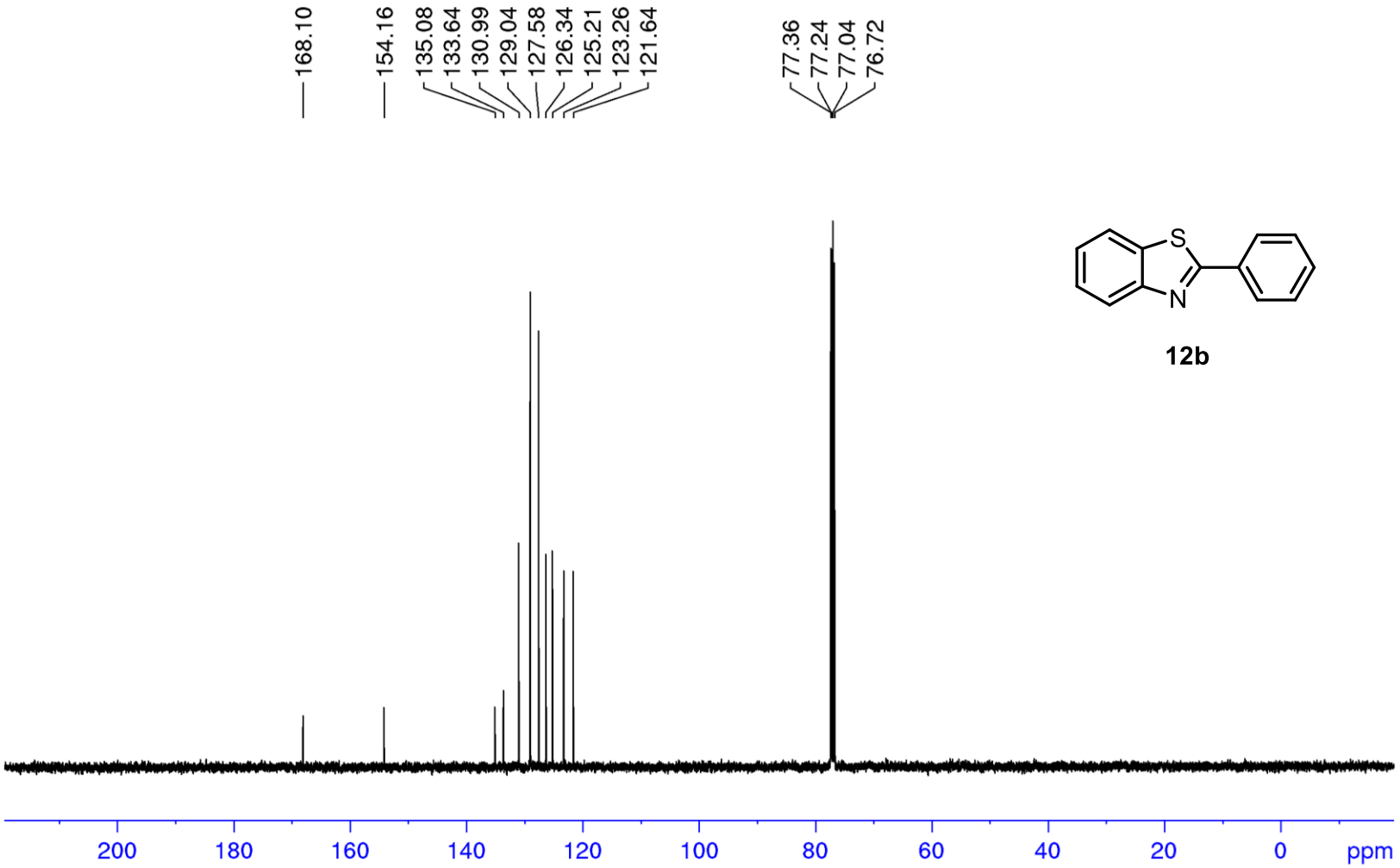
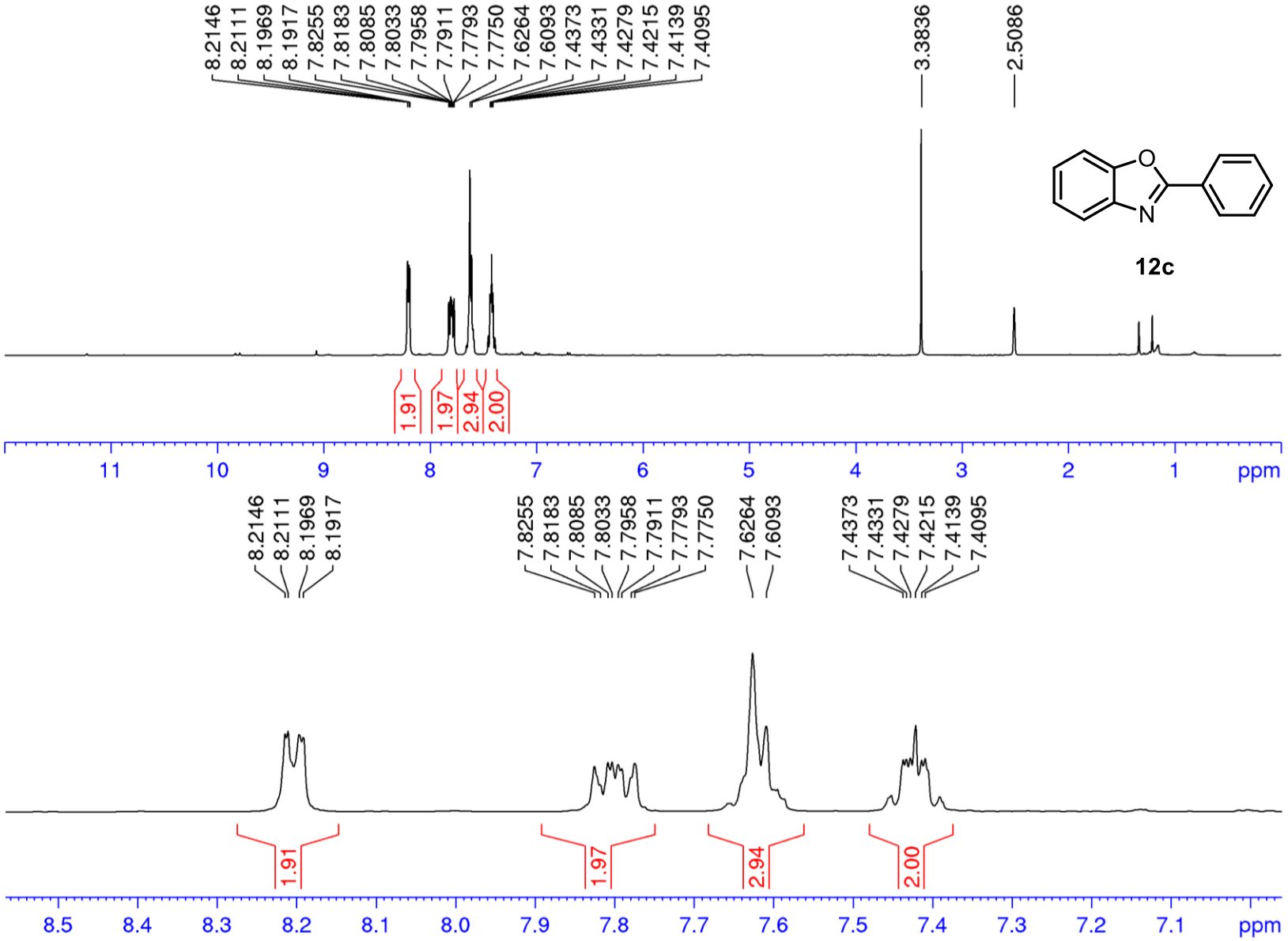
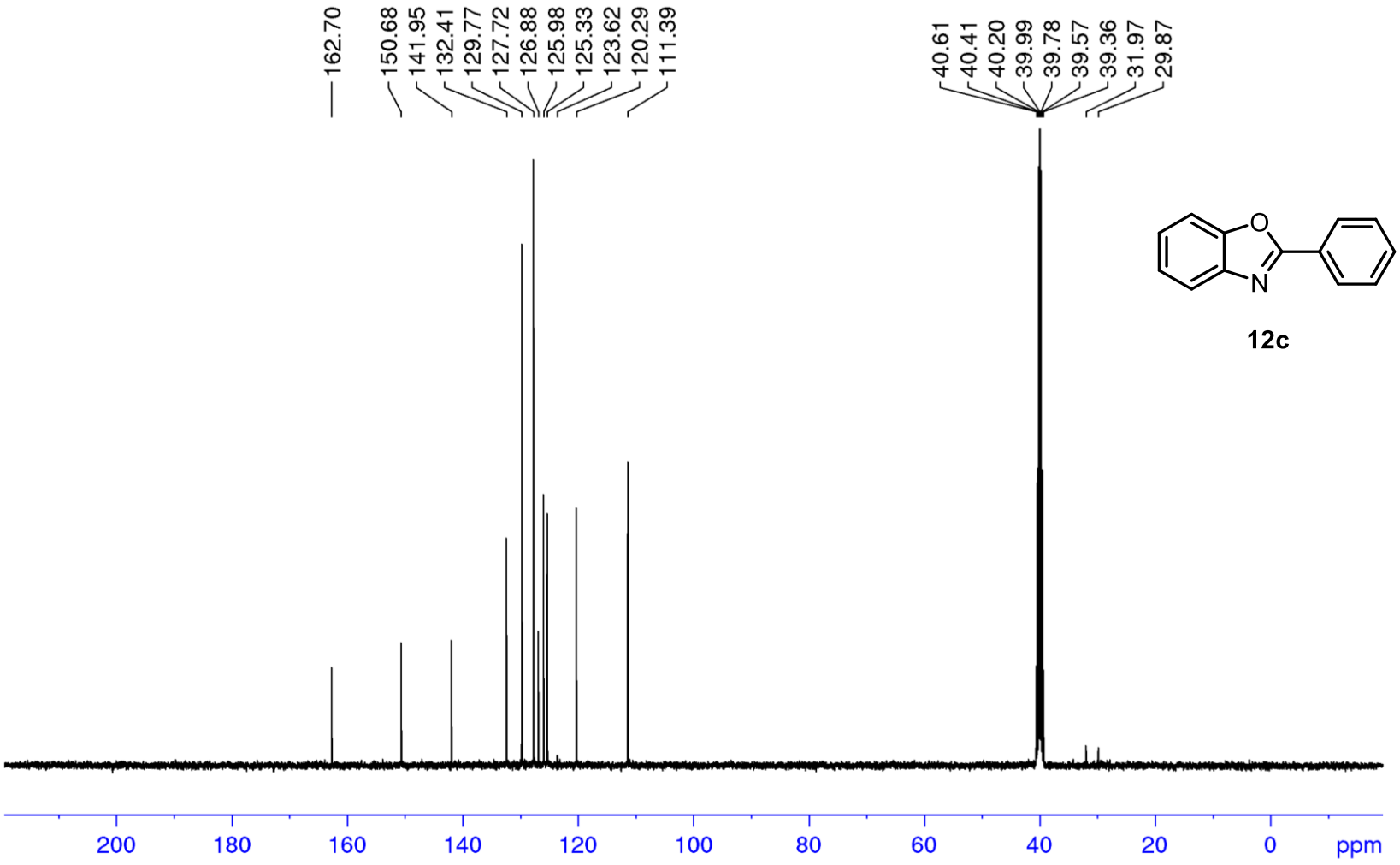
8.1200
8.1138
8.1073
8.1004
7.9493
7.9483
7.9293
7.9283
7.5611
7.5472
7.5437
7.5360
7.5268
7.5197
7.5091
7.5060
7.4396
7.4369
7.4194
7.4017
7.3989
7.2848
S
N
12b
2.94
0.99
3.95
1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm

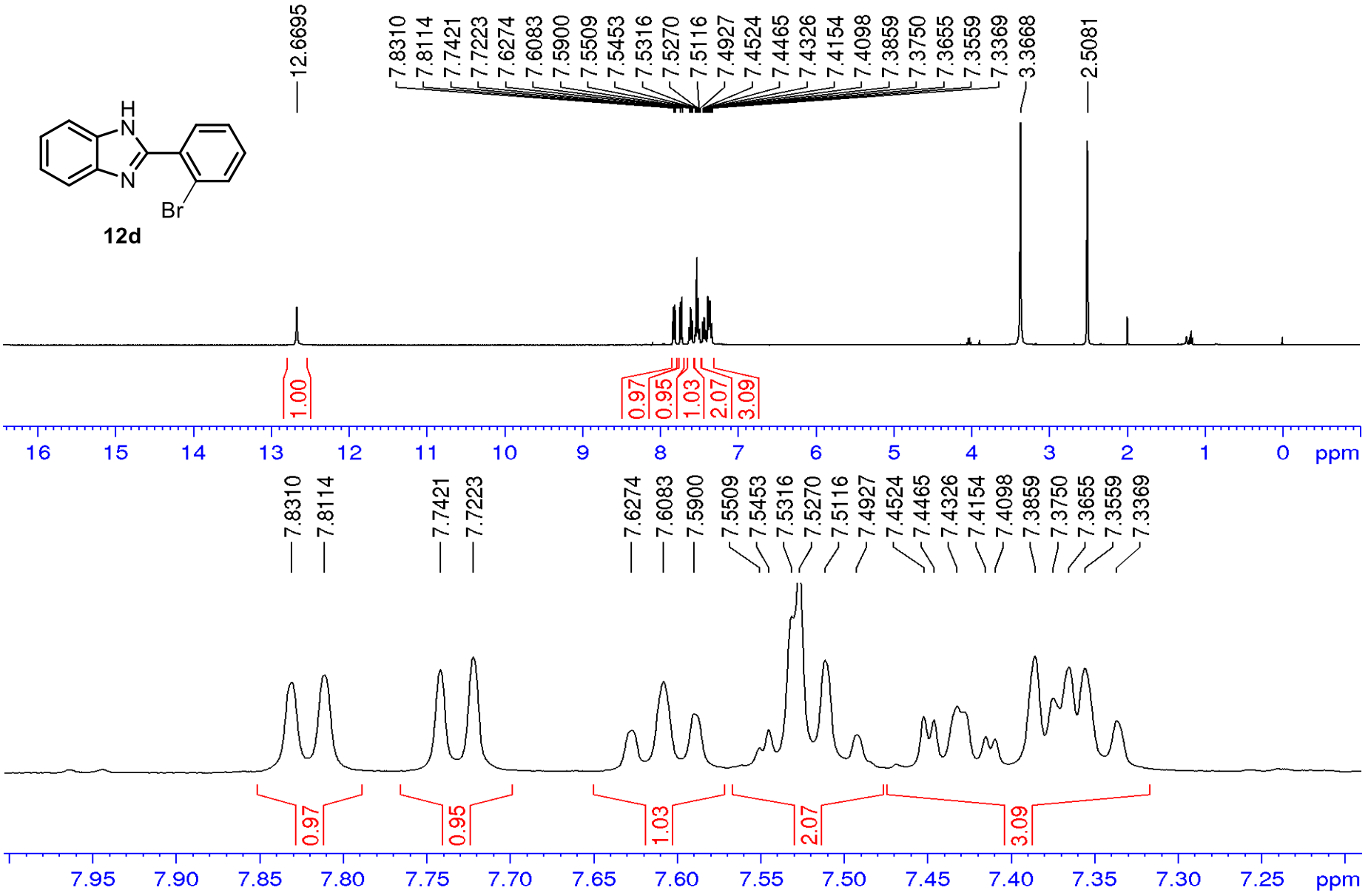

168.10
154.16
135.08
133.64
130.99
129.04
127.58
126.34
125.21
123.26
121.64
77.36
77.24
77.04
76.72
S
N
200
180
160
140
120
100
80
60
40
20
0
ppm

**12b**

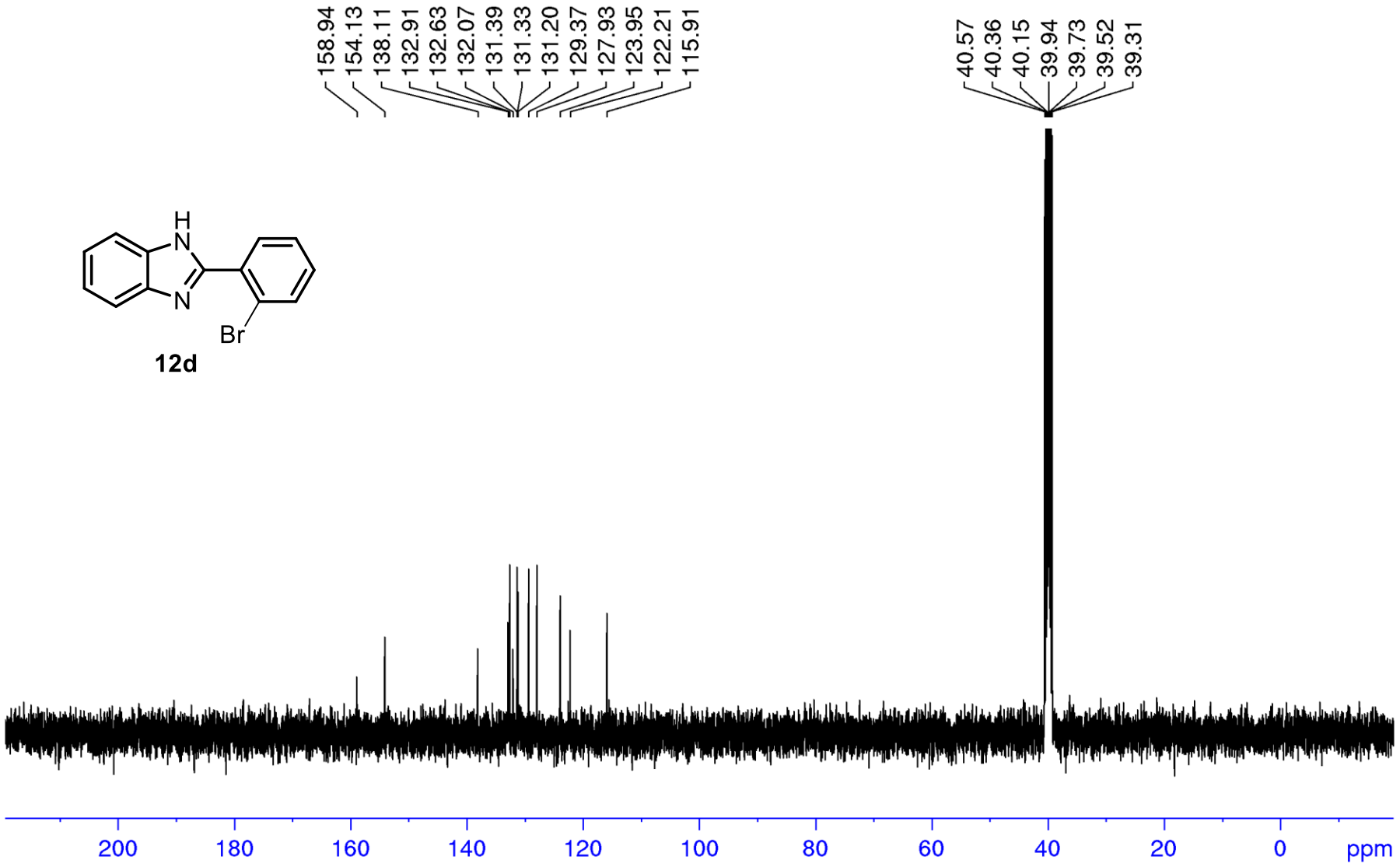

8.2146
8.2111
8.1969
8.1917
7.8255
7.8183
7.8085
7.8033
7.7958
7.7911
7.7793
7.7750
7.6264
7.6093
7.4373
7.4331
7.4279
7.4215
7.4139
7.4095
3.3836
2.5086
O
N
12c
1.91
1.97
2.94
2.00
11
10
9
8
7
6
5
4
3
2
1
ppm
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm


162.70
150.68
141.95
132.41
129.77
127.72
126.88
125.98
125.33
123.62
120.29
111.39
40.61
40.41
40.20
39.99
39.78
39.57
39.36
31.97
29.87
O
N
200
180
160
140
120
100
80
60
40
20
0
ppm

**12c**


12.6695
7.8310
7.8114
7.7421
7.7223
7.6274
7.6083
7.5900
7.5509
7.5453
7.5316
7.5270
7.5116
7.4927
7.4524
7.4465
7.4326
7.4154
7.4098
7.3859
7.3750
7.3655
7.3559
7.3369
3.3668
2.5081
1.00
0.97
0.95
1.03
2.07
3.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 ppm

**12d**


158.94
154.13
138.11
132.91
132.63
132.07
131.39
131.33
131.20
129.37
127.93
123.95
122.21
115.91
40.57
40.36
40.15
39.94
39.73
39.52
39.31
H
N
N
Br
12d
200
180
160
140
120
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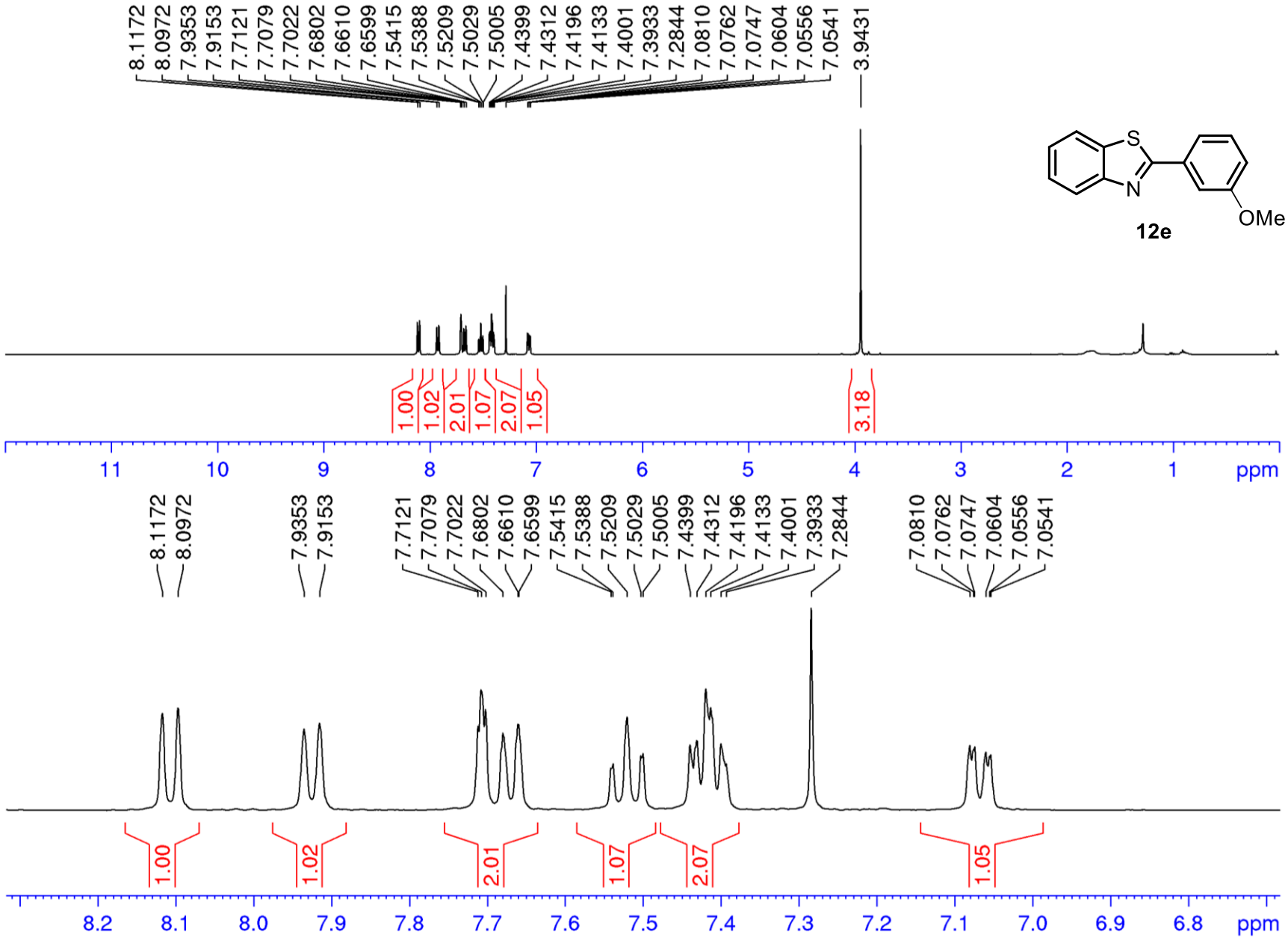
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7.5388
7.5209
7.5029
7.5005
7.4399
7.4312
7.4196
7.4133
7.4001
7.3933
7.2844
7.0810
7.0762
7.0747
7.0604
7.0556
7.0541
3.9431
S
N
OMe
12e
1.00
1.02
2.01
1.07
2.07
1.05
3.18
11
10
9
8
7
6
5
4
3
2
1
ppm
8.2
8.1
8.0
7.9
7.8
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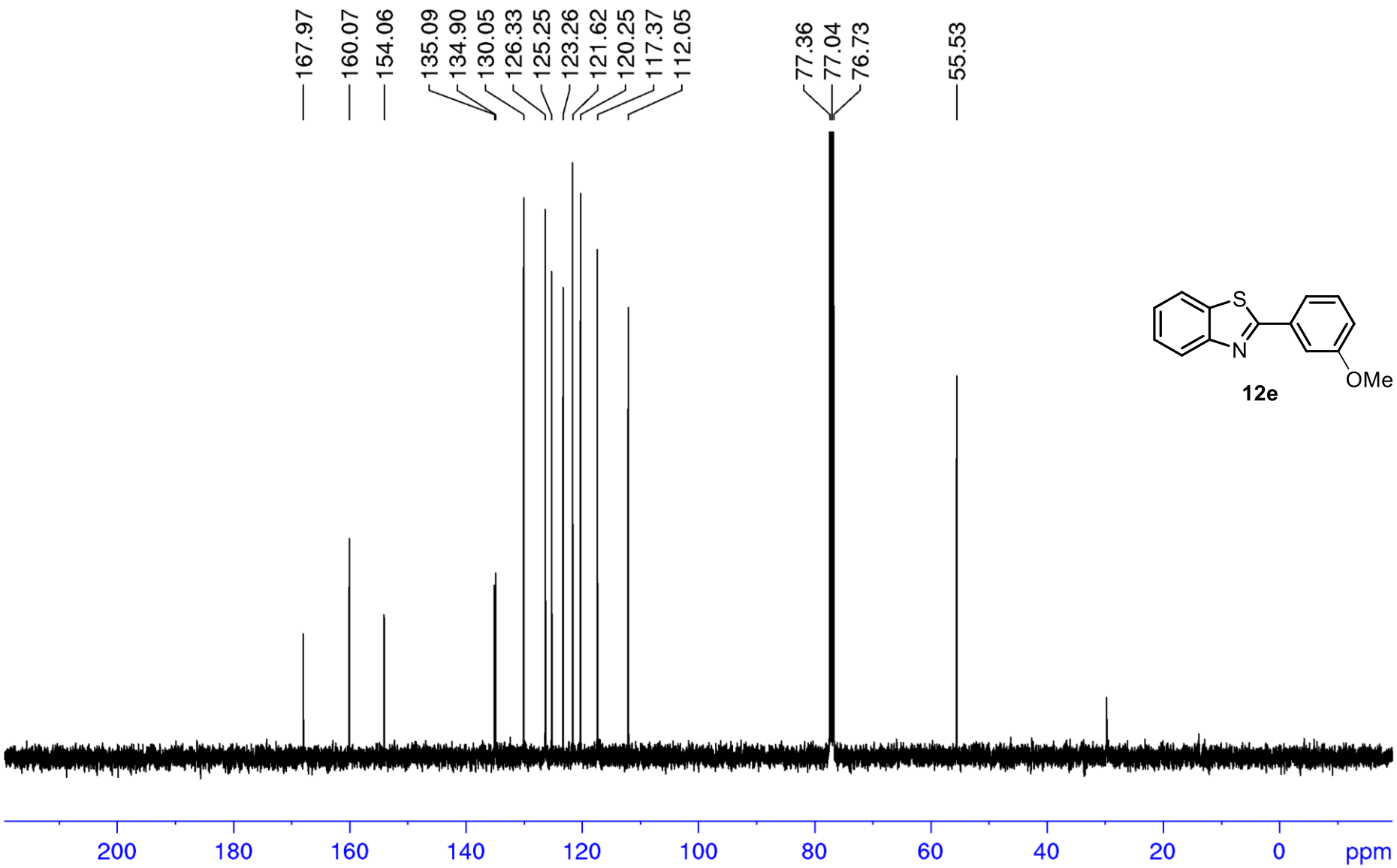
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm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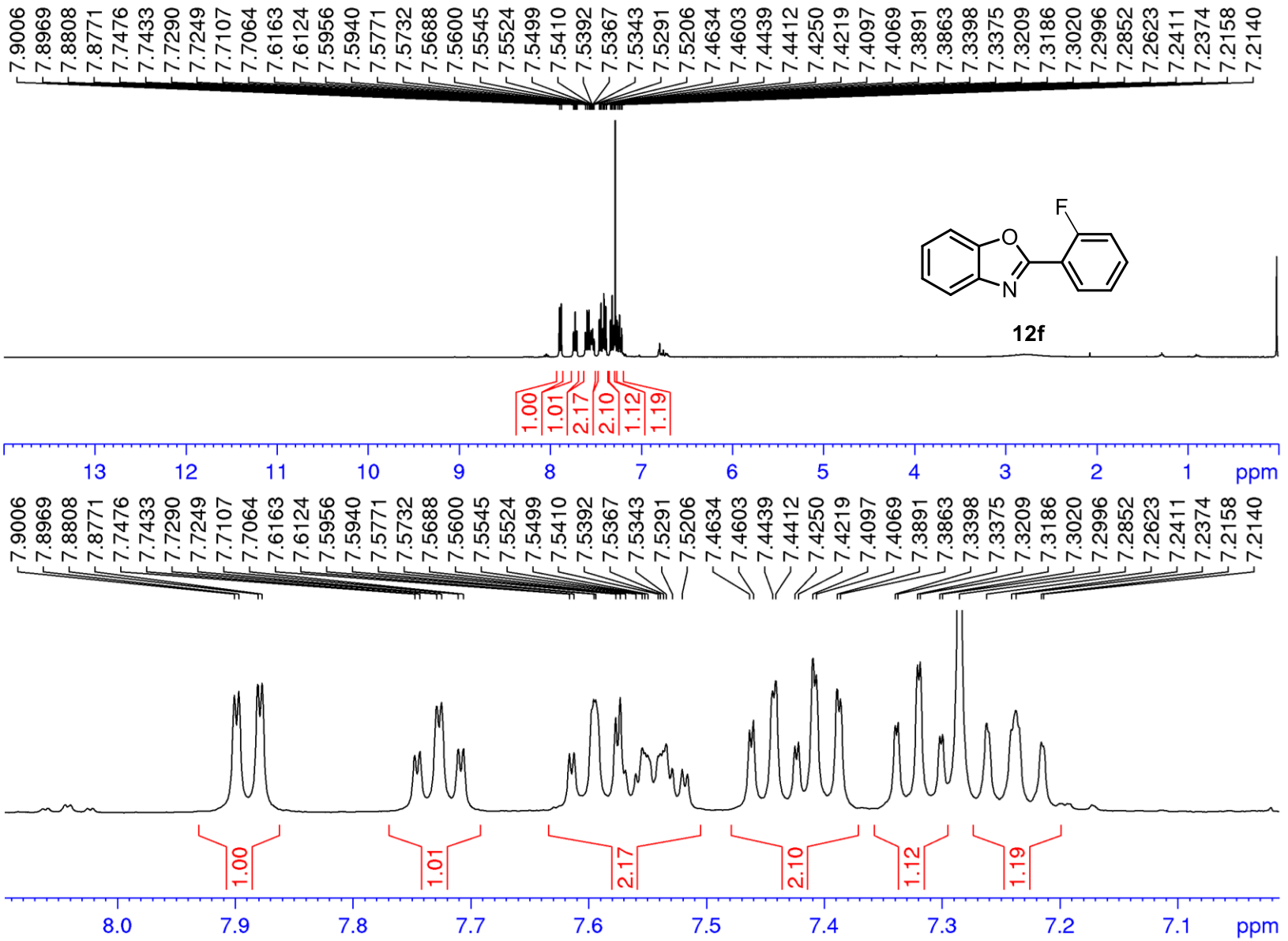
154.06
135.09
134.90
130.05
126.33
125.25
123.26
121.62
120.25
117.37
112.05
77.36
77.04
76.73
55.53
S
N
OMe
12e
200
180
160
140
120
100
80
60
40
20
0
ppm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7.7290
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7.7107
7.7064
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7.6124
7.5956
7.5940
7.5771
7.5732
7.5688
7.5600
7.5545
7.5524
7.5499
7.5410
7.5392
7.5367
7.5343
7.5291
7.5206
7.4634
7.4603
7.4439
7.4412
7.4250
7.4219
7.4097
7.4069
7.3891
7.3863
7.3398
7.3375
7.3209
7.3186
7.3020
7.2996
7.2852
7.2623
7.2411
7.2374
7.2158
7.2140
F
O
N
12f
1.00
1.01
2.17
2.10
1.12
1.19
13
12
11
10
9
8
7
6
5
4
3
2
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ppm
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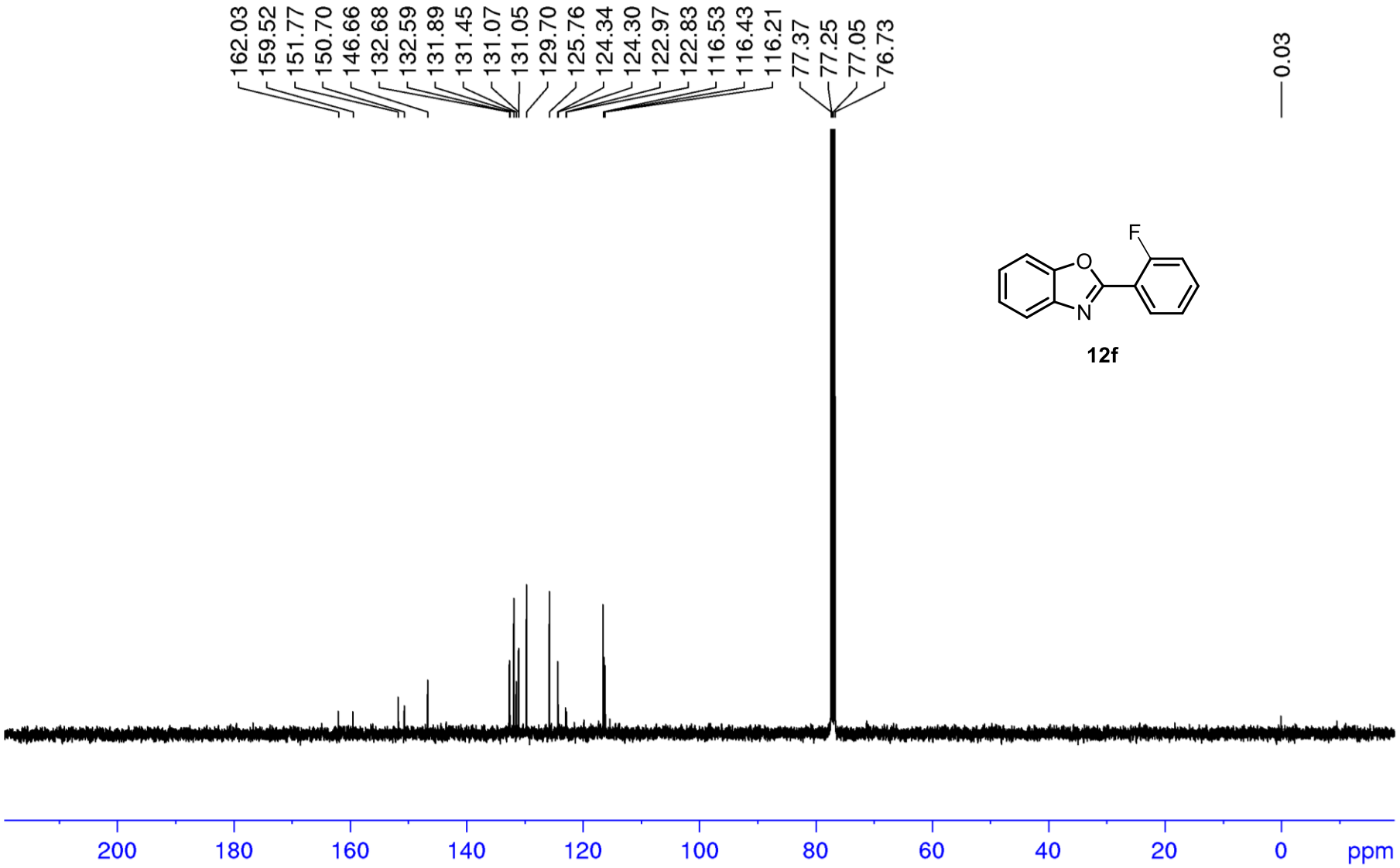
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm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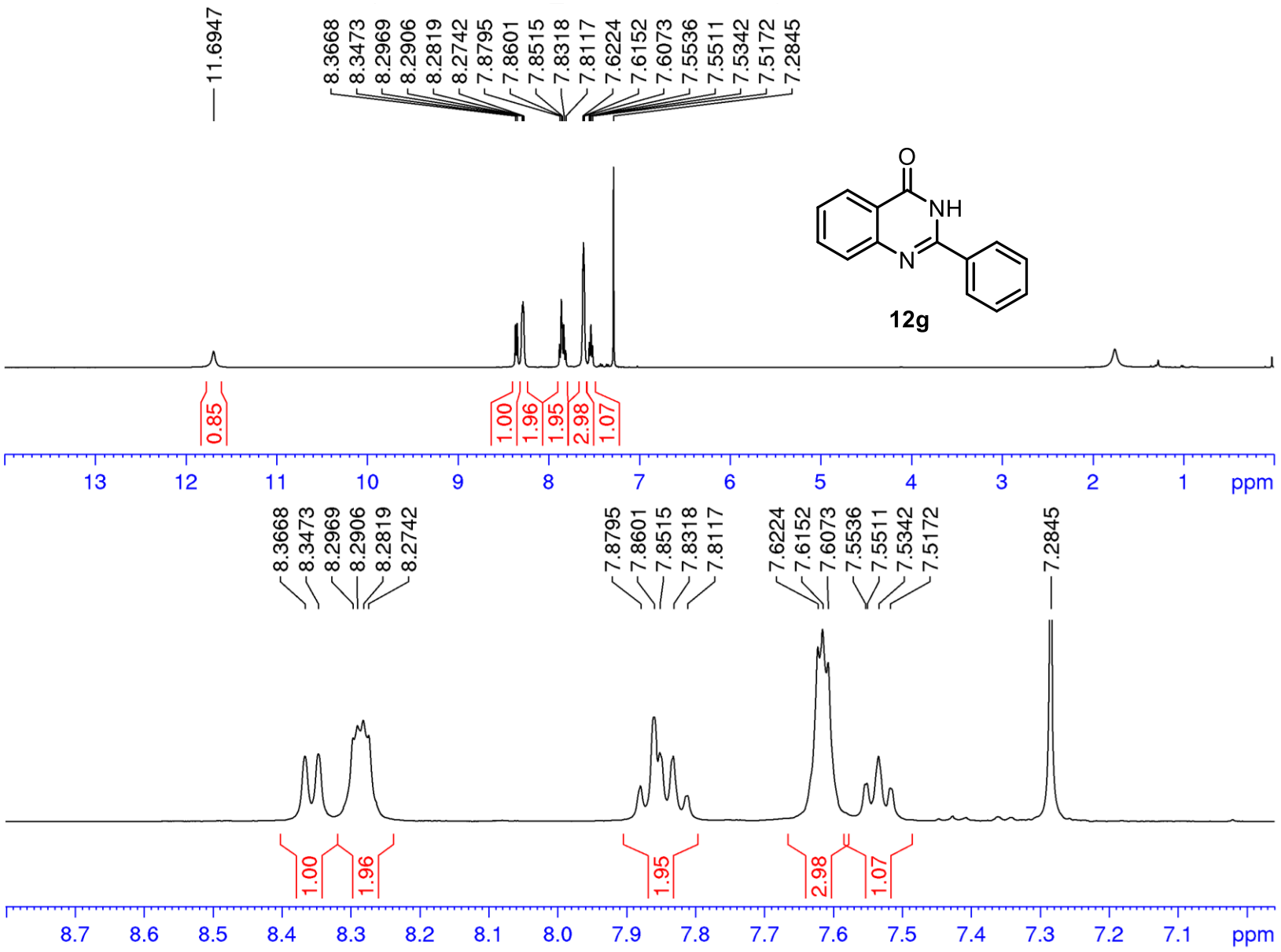
159.52
151.77
150.70
146.66
132.68
132.59
131.89
131.45
131.07
131.05
129.70
125.76
124.34
124.30
122.97
122.83
116.53
116.43
116.21
77.37
77.25
77.05
76.73
0.03
F
O
N
12f
200
180
160
140
120
100
80
60
40
20
0
ppm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8.2742
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7.8601
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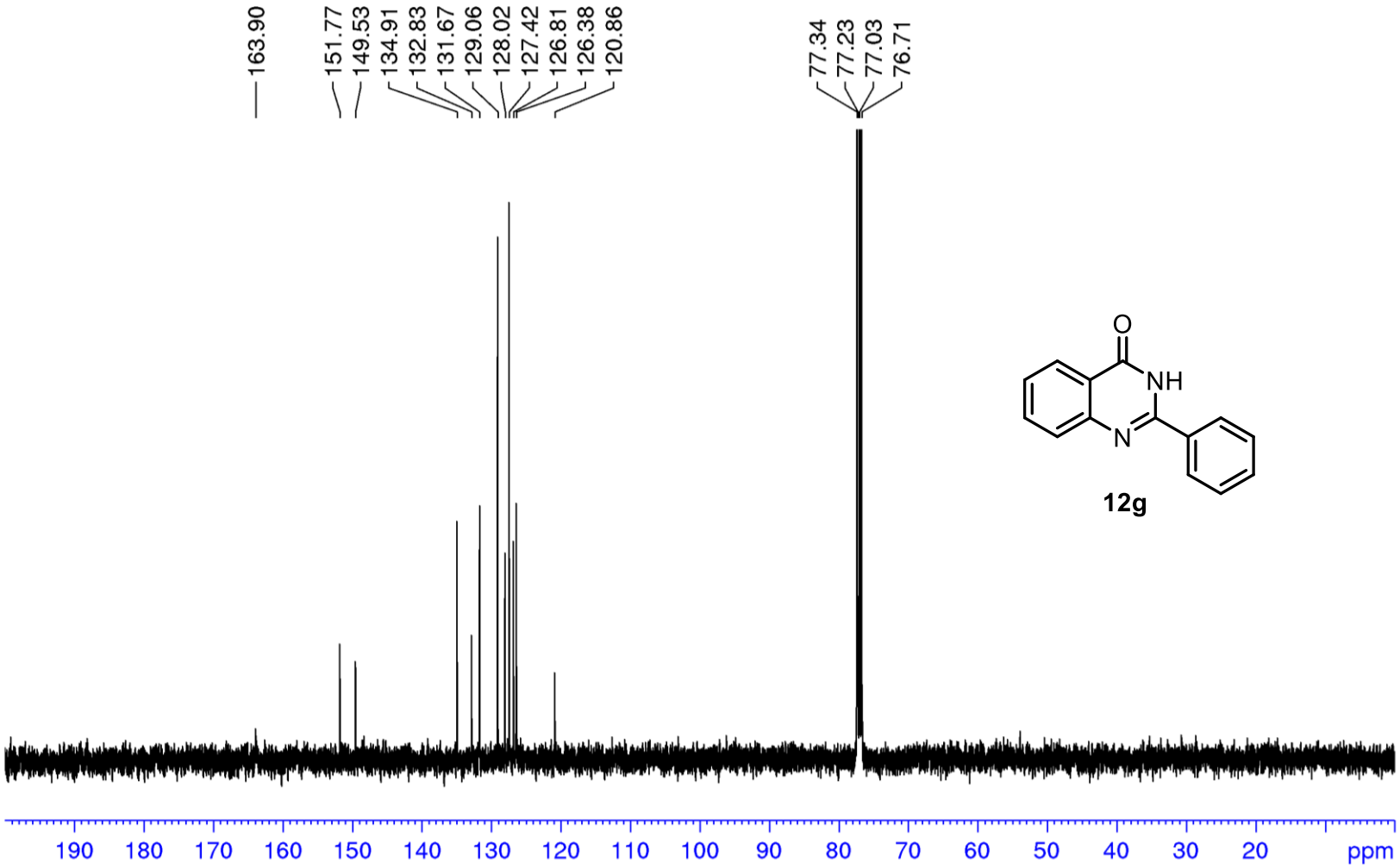
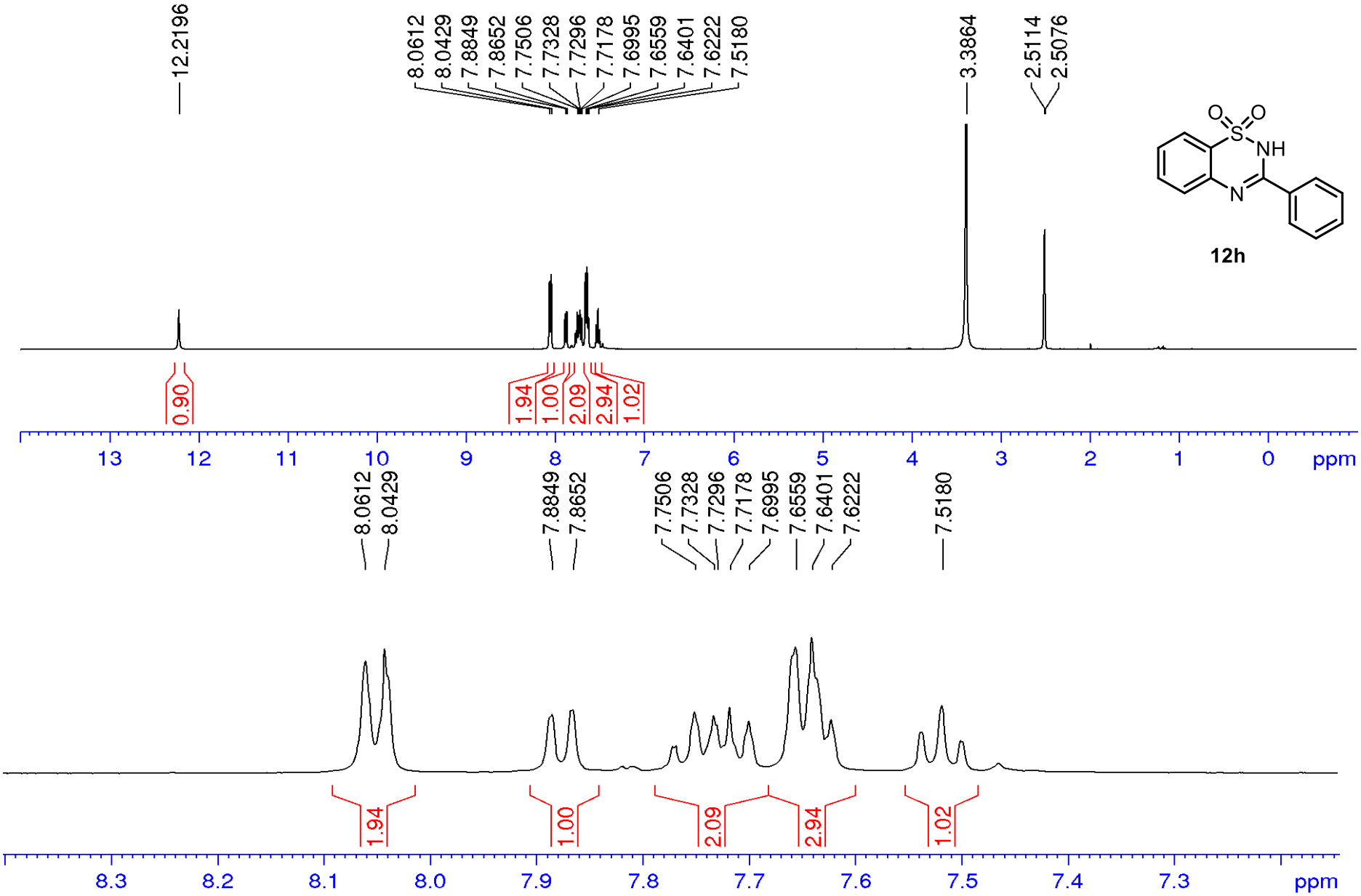
7.8318
7.8117
7.6224
7.6152
7.6073
7.5536
7.5511
7.5342
7.5172
7.2845
O
NH
N
12g
0.85
1.00
1.96
1.95
2.98
1.07
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm


163.90
151.77
149.53
134.91
132.83
131.67
129.06
128.02
127.42
126.81
126.38
120.86
77.34
77.23
77.03
76.71
O
NH
N
12g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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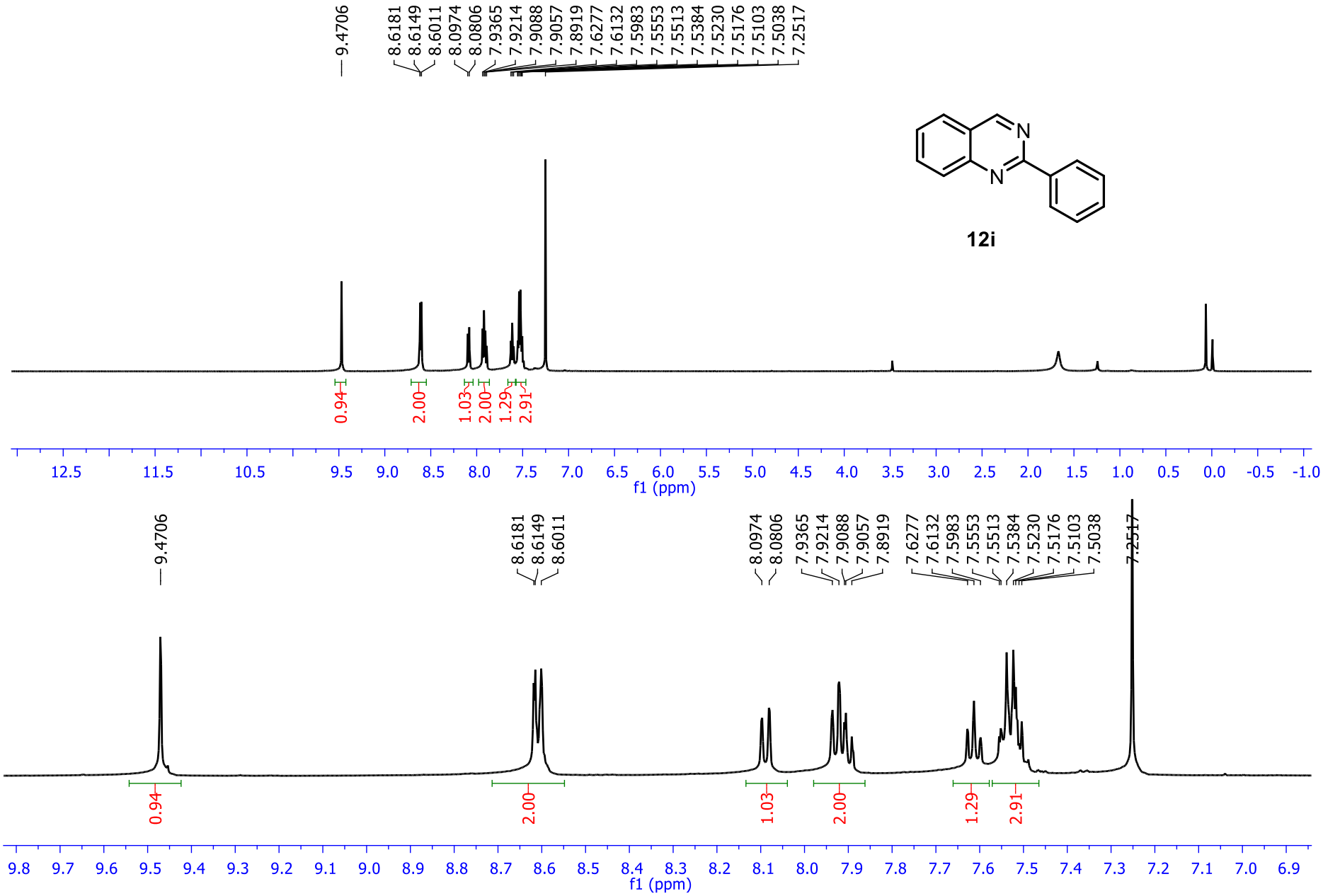
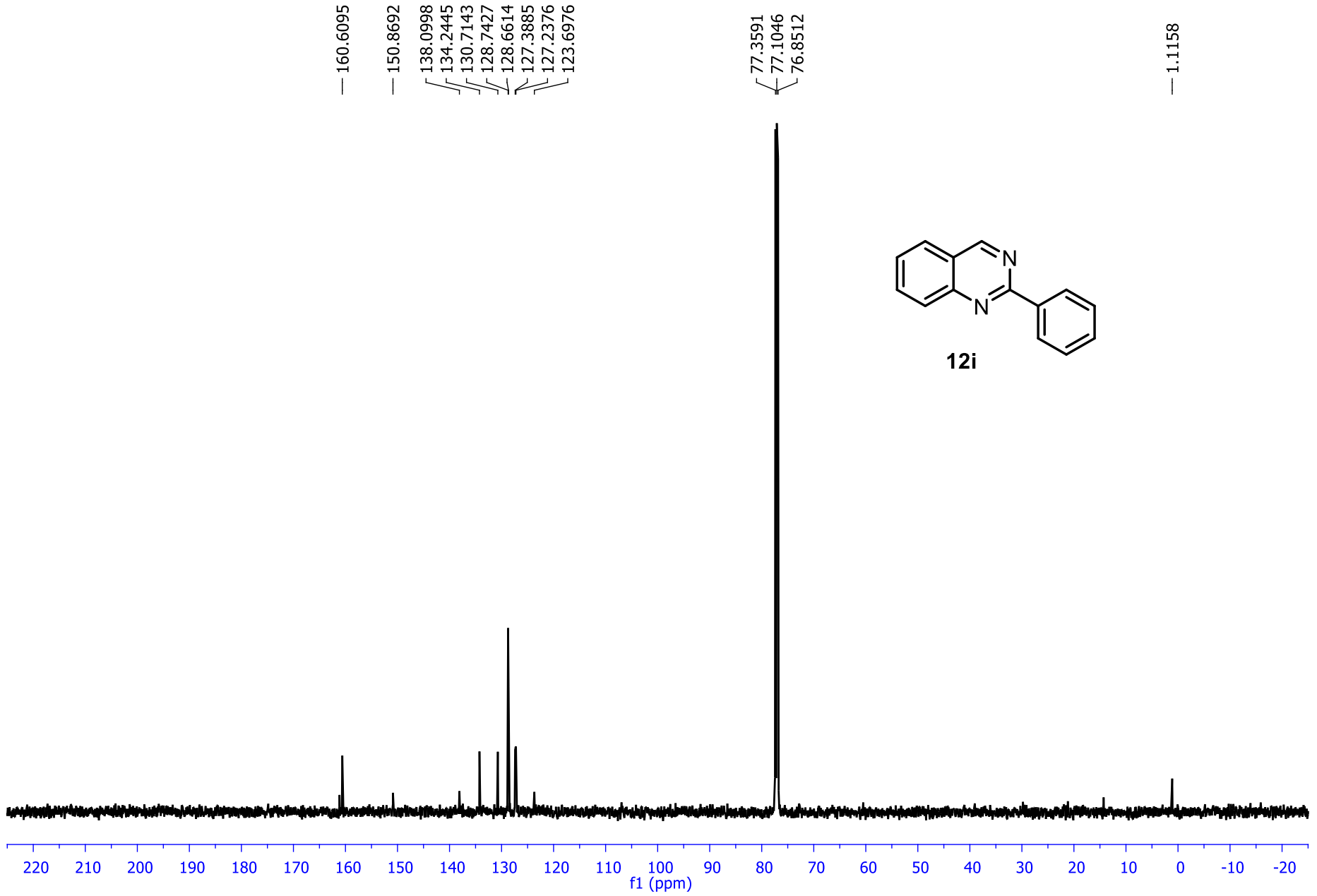
8.0612
8.0429
7.8849
7.8652
7.7506
7.7328
7.7296
7.7178
7.6995
7.6559
7.6401
7.6222
7.5180
3.3864
2.5114
2.5076
O
O
S
NH
N
12h
0.90
1.94
1.00
2.09
2.94
1.02
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
8.0612
8.0429
7.8849
7.8652
7.7506
7.7328
7.7296
7.7178
7.6995
7.6559
7.6401
7.6222
7.5180
1.94
1.00
2.09
2.94
1.02
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm


9.4706
8.6181
8.6149
8.6011
8.0974
8.0806
7.9365
7.9214
7.9088
7.9057
7.8919
7.6277
7.6132
7.5983
7.5553
7.5513
7.5384
7.5230
7.5176
7.5103
7.5038
7.2517
N
N
12i
0.94
2.00
1.03
2.00
1.29
2.91
f1 (ppm)
9.4706
8.6181
8.6149
8.6011
8.0974
8.0806
7.9365
7.9214
7.9088
7.9057
7.8919
7.6277
7.6132
7.5983
7.5553
7.5513
7.5384
7.5230
7.5176
7.5103
7.5038
7.2517
0.94
2.00
1.03
2.00
1.29
2.91
f1 (ppm)


160.6095
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130.7143
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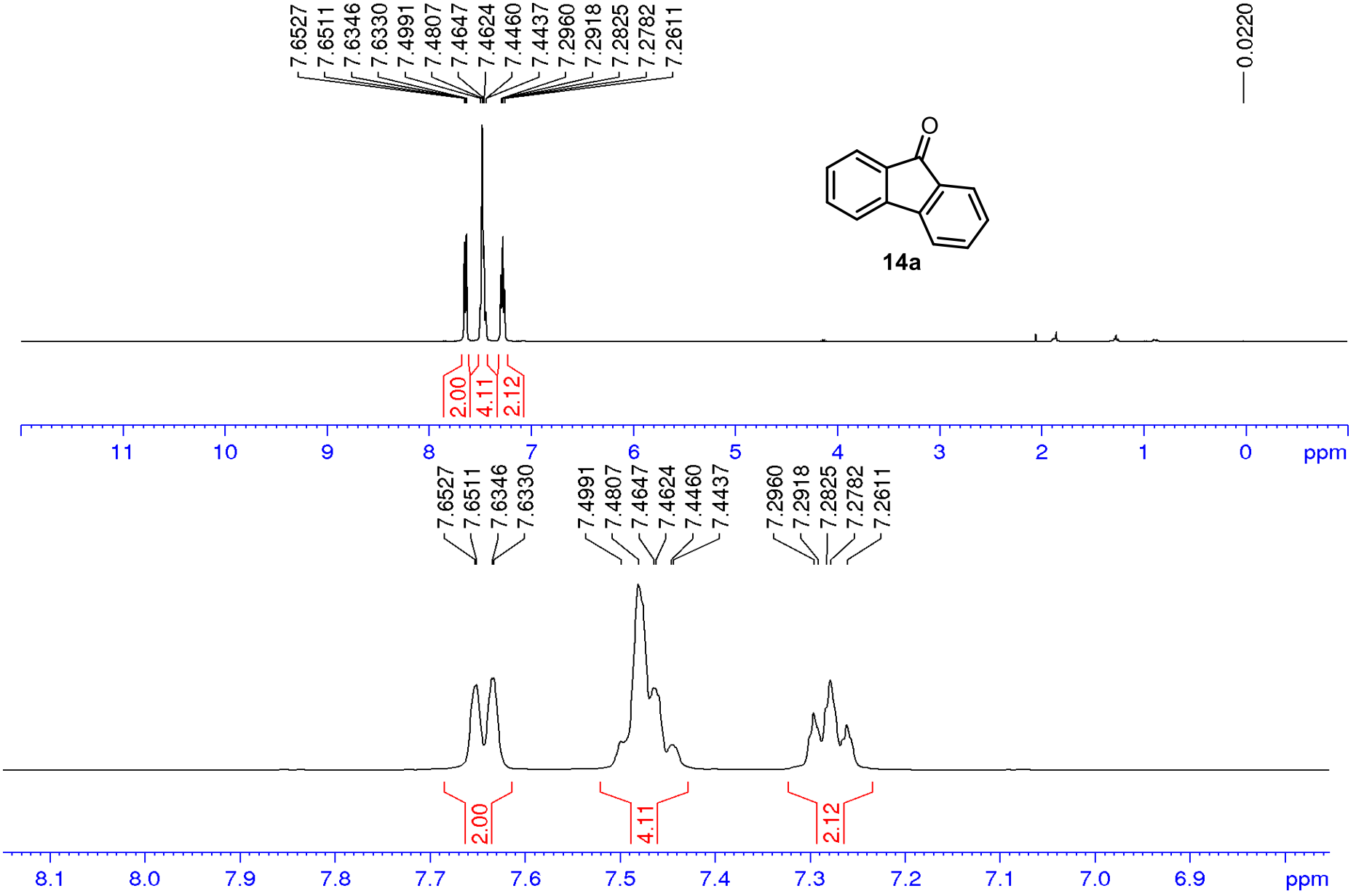
127.3885
127.2376
123.6976
77.3591
77.1046
76.8512
1.1158
N
N
12i
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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7.4991
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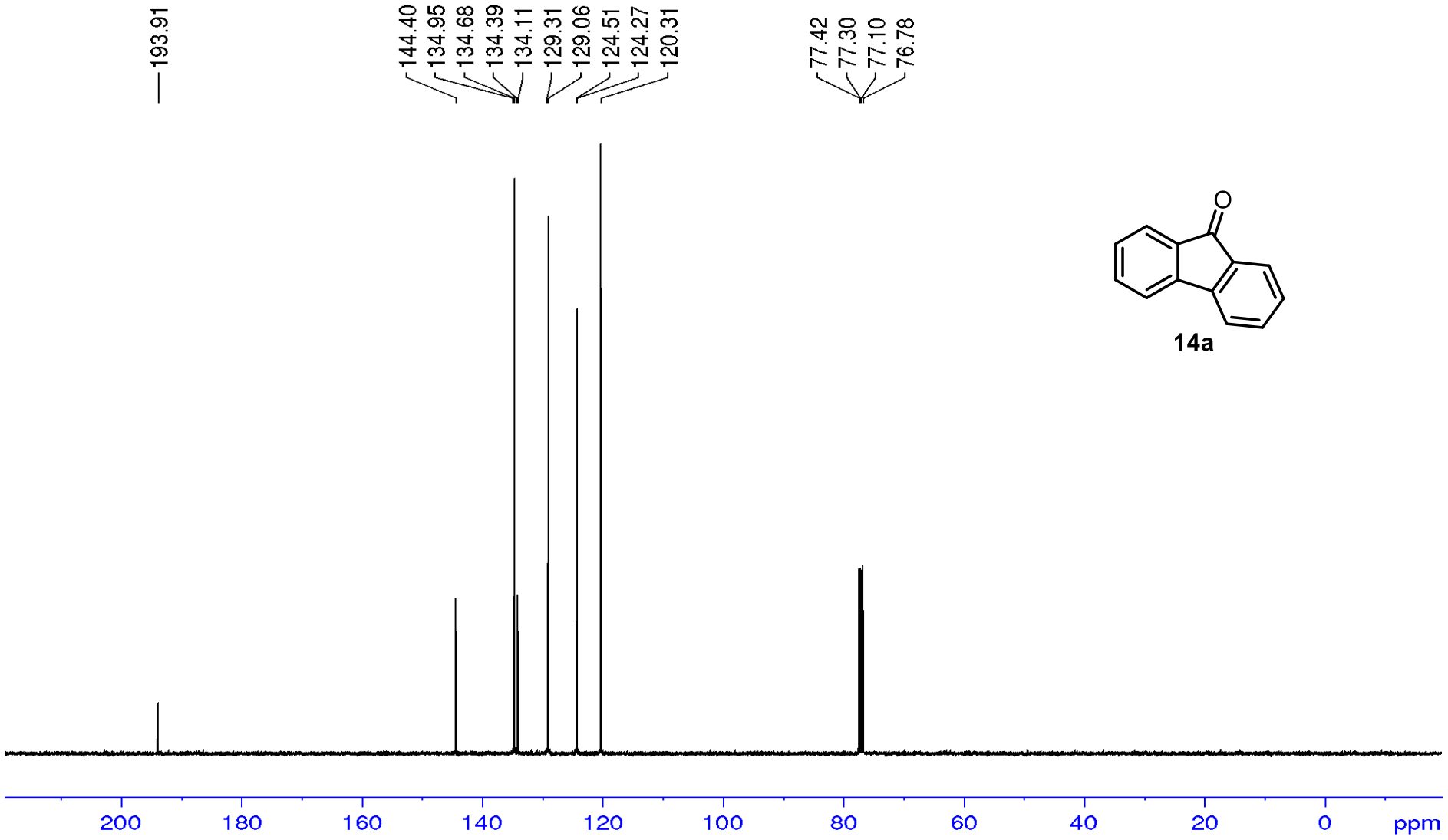
7.4647
7.4624
7.4460
7.4437
7.2960
7.2918
7.2825
7.2782
7.2611
0.0220
O
14a
2.00
4.11
2.12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm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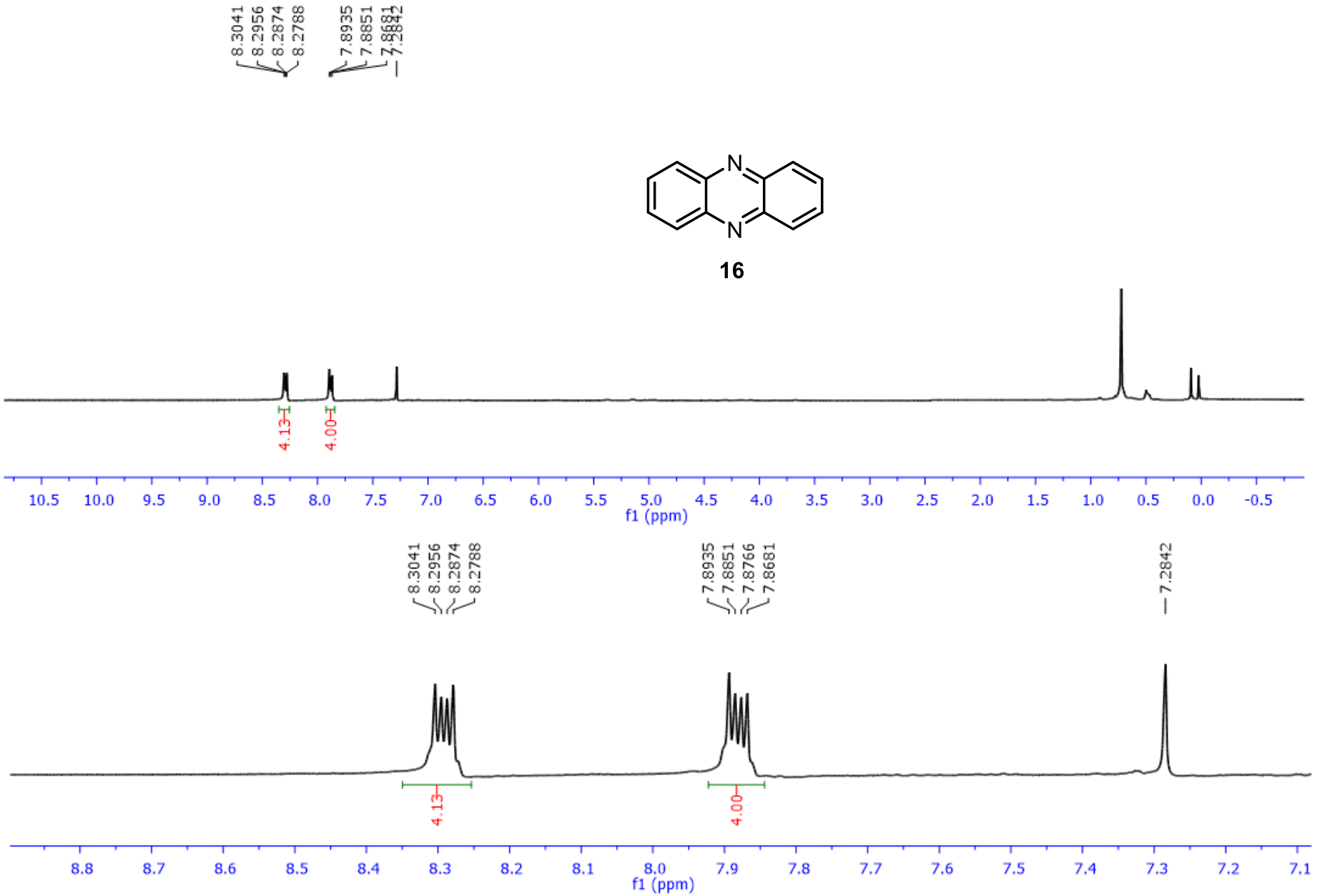
134.68
134.39
134.11
129.31
129.06
124.51
124.27
120.31
77.42
77.30
77.10
76.78
O
14a
200
180
160
140
120
100
80
60
40
20
0
ppm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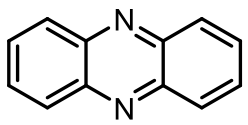
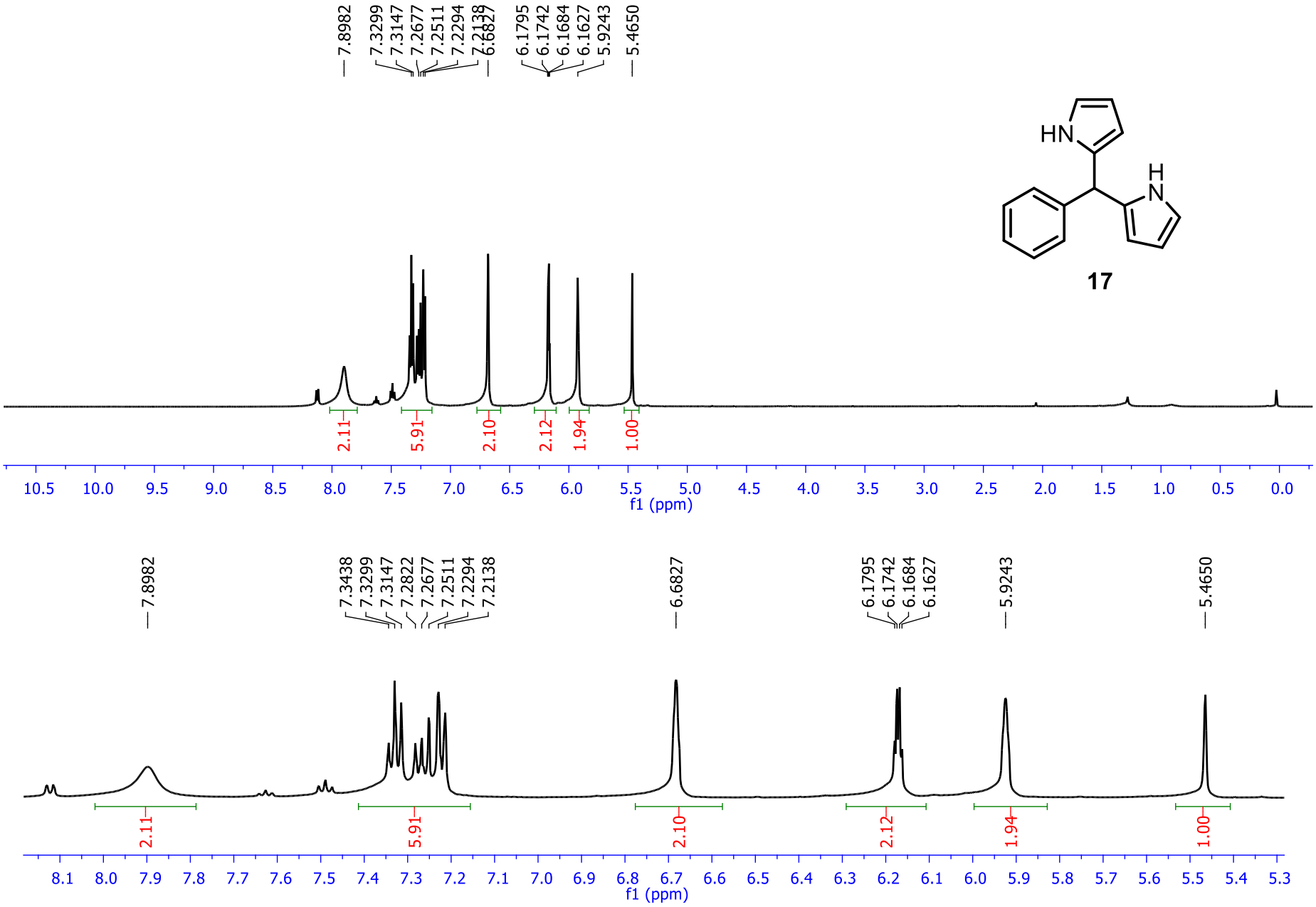
8.2956
8.2874
8.2788
7.8935
7.8851
7.8681
7.2842
N
N
16
4.13
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
8.3041
8.2956
8.2874
8.2788
7.8935
7.8851
7.8766
7.8681
7.2842
4.13
4.00
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)



**16**


143.5383
130.5103
129.6849
77.3313
77.0137
76.6961
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2511
7.2294
7.2138
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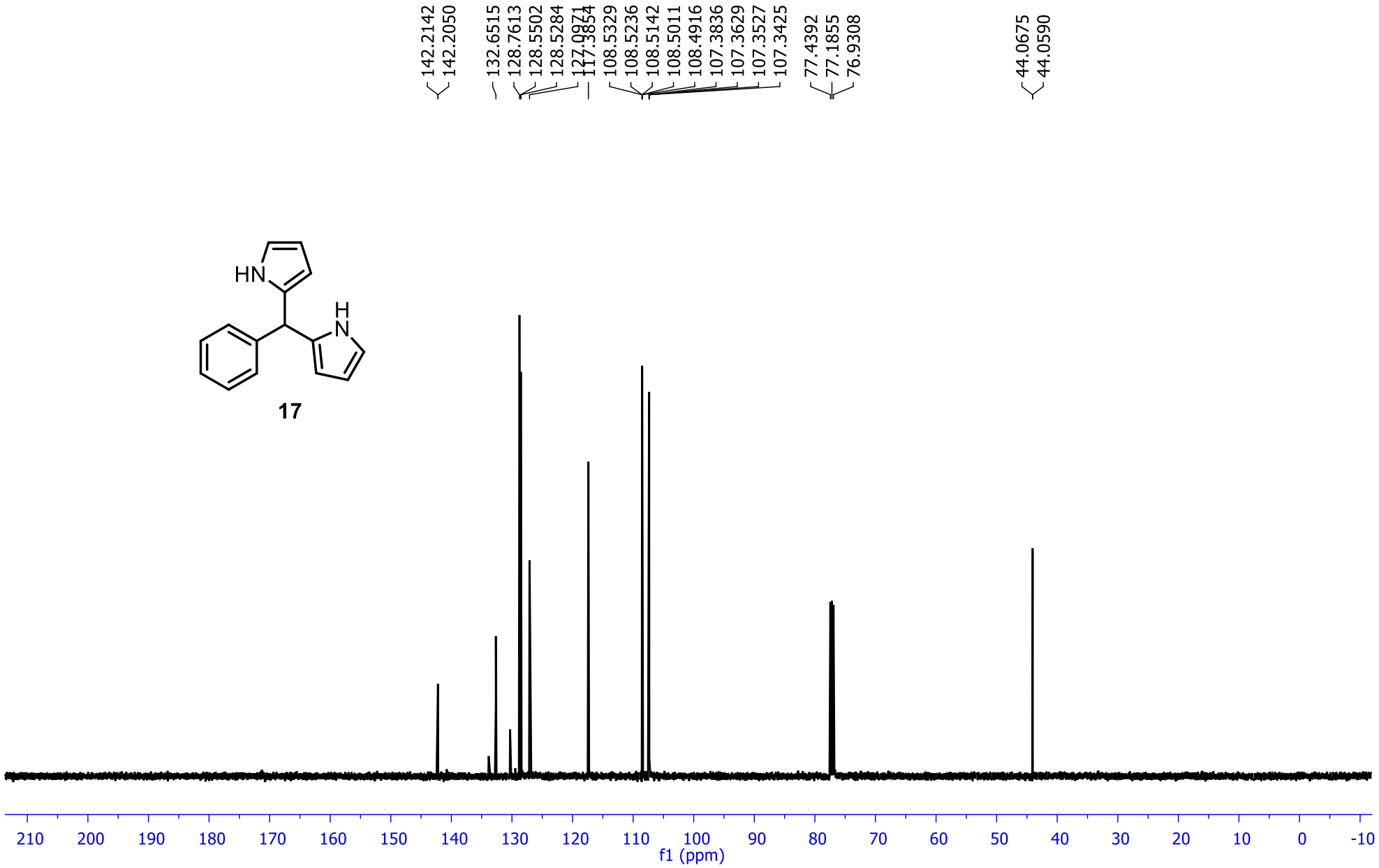
6.1795
6.1742
6.1684
6.1627
5.9243
5.4650
HN
H
N
17
2.11
5.91
2.10
2.12
1.94
1.00
f1 (ppm)
7.8982
7.3438
7.3299
7.3147
7.2822
7.2677
7.2511
7.2294
7.2138
6.6827
6.1795
6.1742
6.1684
6.1627
5.9243
5.4650
2.11
5.91
2.10
2.12
1.94
1.00
f1 (ppm)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127.0971
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108.5329
108.5236
108.5142
108.5011
108.4916
107.3836
107.3629
107.3527
107.3425
77.4392
77.1855
76.9308
44.0675
44.0590
HN
H
N
17
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)